

# Sparse/Robust Estimation and Kalman Smoothing with Nonsmooth Log-Concave Densities: Modeling, Computation, and Theory

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**Abstract**

We introduce a class of quadratic support (QS) functions, many of which already play a crucial role in a variety of applications, including machine learning, robust statistical inference, sparsity promotion, and inverse problems such as Kalman smoothing. Well known examples of QS penalties include the  $\ell_2$ , Huber,  $\ell_1$  and Vapnik losses. This paper builds on a dual representation for QS functions using convex analysis. The dual representation reveals the structure necessary for a QS function to be interpreted as the negative log of a true probability density, and thus provides the foundation for statistical interpretation and analysis of both known and new QS loss functions. Moreover, in some cases, it allows for the construction of non-smooth multivariate distributions with specified means and variances from simple scalar building blocks. Finally, for a broad subclass of QS loss functions known as piecewise linear quadratic (PLQ) penalties, it is shown how the dual representation allows for the development of efficient numerical estimation schemes. The main contribution of this paper is a flexible statistical modeling framework for a variety of learning applications, together with a toolbox of efficient numerical methods for estimation using these densities. In particular, for PLQ densities, we show that interior point (IP) methods can be used. IP methods solve nonsmooth optimization problems by working directly with smooth systems of equations characterizing the optimality of these problems. The efficiency of the IP approach depends on the structure of particular applications. We consider the class of dynamic inverse problems using Kalman smoothing. This class comprises a wide variety of applications, where the aim is to reconstruct the state of a dynamical system with known process and measurement models starting from noisy output samples. In the classical case, Gaussian errors are assumed both in the process and measurement models for such problems. The extended framework allows arbitrary PLQ densities to be used, and the proposed IP approach solves the generalized Kalman smoothing problem while maintaining the linear complexity in the size of the time series, just as in the Gaussian case. This extends the computational efficiency of the Mayne-Fraser and Rauch-Tung-Striebel algorithms to a much broader nonsmooth setting, and includes many recently proposed robust and sparse smoothers as special cases.

**Keywords:** statistical modeling; convex analysis; nonsmooth optimization; robust inference; sparsity optimization; Kalman smoothing; interior point methods

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## 1. Introduction

Consider the classical problem of Bayesian parametric regression (MacKay, 1992; Roweis and Ghahramani, 1999) where the unknown  $x \in \mathbb{R}^n$  is a random vector<sup>1</sup>, with a prior distribution specified using a known invertible matrix  $G \in \mathbb{R}^{n \times n}$  and known vector  $\mu \in \mathbb{R}^n$  via

$$\mu = Gx + w, \quad (1.1) \text{?LinearProcess?}$$

where  $w$  is a zero mean vector with covariance  $Q$ . Let  $z$  denote a linear transformation of  $x$  contaminated with additive zero mean measurement noise  $v$  with covariance  $R$ ,

$$z = Hx + v, \quad (1.2) \text{?LinearModel?}$$

where  $H \in \mathbb{R}^{\ell \times n}$  is a known matrix, while  $v$  and  $w$  are independent. It is well known that the (unconditional) minimum variance linear estimator of  $x$ , as a function of  $z$ , is the solution to the following optimization problem:

$$\min_x (z - Hx)^T R^{-1} (z - Hx) + (\mu - Gx)^T Q^{-1} (\mu - Gx). \quad (1.3) \text{?MainObjective?}$$

As we will show, (1.3) includes estimation problems arising in discrete-time dynamic linear systems which admit a state space representation (Anderson and Moore, 1979; Brockett, 1970). In this context,  $x$  is partitioned into  $N$  subvectors  $\{x_k\}$ , where each  $x_k$  represents the hidden system state at time instant  $k$ . For known data  $z$ , the classical Kalman smoother exploits the special structure of the matrices  $H, G, Q$  and  $R$  to compute the solution of (1.3) in  $O(N)$  operations (Gelb, 1974). This procedure returns the minimum variance estimate of the state sequence  $\{x_k\}$  when the additive noise in the system is assumed to be Gaussian.

In many circumstances, the estimator (1.3) performs poorly; put another way, quadratic penalization on model deviation is a bad model in many situations. For instance, it is not robust with respect to the presence of outliers in the data (Huber, 1981; Gao, 2008; Aravkin et al., 2011a; Farahmand et al., 2011) and may have difficulties in reconstructing fast system dynamics, e.g. jumps in the state values (Ohlsson et al., 2011). In addition, sparsity-promoting regularization is often used in order to extract a small subset from a large measurement or parameter vector which has greatest impact on the predictive capability of the estimate for future data. This sparsity principle permeates many well known techniques in machine learning and signal processing, including feature selection, selective shrinkage, and compressed sensing (Hastie and Tibshirani, 1990; Efron et al., 2004; Donoho, 2006). In these cases, (1.3) is often replaced by a more general formulation

$$\min_x V(Hx - z; R) + W(Gx - \mu; Q) \quad (1.4) \text{?probTwo?}$$

where the loss  $V$  may be the  $\ell_2$ -norm, the Huber penalty (Huber, 1981), Vapnik's  $\varepsilon$ -insensitive loss (used in support vector regression (Vapnik, 1998) see also (Hastie et al., 2001)) or the hinge loss (leading to support vector classifiers (Evgeniou et al., 2000; Pontil and Verri, 1998; Schölkopf et al., 2000)). The regularizer  $W$  may be the  $\ell_2$ -norm, the  $\ell_1$ -norm (as in the LASSO (Tibshirani, 1996)), or a weighted combination of the two, yielding the elastic net procedure (Zou and Hastie, 2005). Many learning algorithms using infinite-dimensional reproducing kernel Hilbert spaces as hypothesis spaces (Aronszajn, 1950; Saitoh, 1988; Cucker and Smale, 2001) boil down to solving

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1. All vectors are column vectors, unless otherwise specified

finite-dimensional problems of the form (1.4) by virtue of the representer theorem (Wahba, 1998; Schölkopf et al., 2001).

These robust and sparse approaches can often be interpreted as placing non-Gaussian priors on  $w$  (or directly on  $x$ ) and on the measurement noise  $v$ . The Bayesian interpretation of (1.4) has been extensively studied in the statistical and machine learning literature in recent years and probabilistic approaches used in the analysis of estimation and learning algorithms can be found e.g. in (Mackay, 1994; Tipping, 2001; Wipf et al., 2011). Non-Gaussian model errors and priors leading to a great variety of loss and penalty functions are also reviewed in (Palmer et al., 2006) using convex-type representations, and integral-type variational representations related to Gaussian scale mixtures.

In contrast to the above approaches, in the first part of the paper, we consider a wide class of quadratic support (QS) functions and exploit their dual representation. This class of functions generalizes the notion of piecewise linear quadratic (PLQ) penalties Rockafellar and Wets (1998). The dual representation is the key to identifying which QS loss functions can be associated with a density, which in turn allows us to interpret the solution to the problem (1.4) as a MAP estimator when the loss functions  $V$  and  $W$  come from this subclass of QS penalties. This viewpoint allows statistical modeling using non-smooth penalties, such as the  $\ell_1$ , hinge, Huber and Vapnik losses, which are all PLQ penalties. Identifying a statistical interpretation for this class of problems gives us several advantages, including a systematic constructive approach to prescribe mean and variance parameters for the corresponding model; a property that is particularly important for Kalman smoothing.

In addition, the dual representation provides the foundation for efficient numerical methods in estimation based on interior point optimization technology. In the second part of the paper, we derive the Karush-Kuhn-Tucker (KKT) equations for problem (1.4), and introduce interior point (IP) methods, which are iterative methods to solve the KKT equations using smooth approximations. This is essentially a smoothing approach to many (non-smooth) robust and sparse problems of interest to practitioners. Furthermore, we provide conditions under which the IP methods solve (1.4) when  $V$  and  $W$  come from PLQ densities, and describe implementation details for the entire class.

A concerted research effort has recently focused on the solution of regularized large-scale inverse and learning problems, where computational costs and memory limitations are critical. This class of problems includes the popular kernel-based methods (Rasmussen and Williams, 2006; Schölkopf and Smola, 2001; Smola and Schölkopf, 2003), coordinate descent methods (Tseng and Yun, 2008; Lucidi et al., 2007; Dinuzzo, 2011) and decomposition techniques (Joachims, 1998; Lin, 2001; Lucidi et al., 2007), one of which is the widely used sequential minimal optimization algorithm for support vector machines (Platt, 1998). Other techniques are based on kernel approximations, e.g. using incomplete Cholesky factorization (Fine and Scheinberg, 2001), approximate eigen-decomposition (Zhang and Kwok, 2010) or truncated spectral representations (Pillonetto and Bell, 2007). Efficient interior point methods have been developed for  $\ell_1$ -regularized problems (Kim et al., 2007), and for support vector machines (Ferris and Munson, 2003).

In contrast, general and efficient solvers for state space estimation problems of the form (1.4) are missing in the literature. The last part of this paper provides a contribution to fill this gap, specializing the general results to the dynamic case, and recovering the classical efficiency results of the least-squares formulation. In particular, we design new Kalman smoothers tailored for systems subject to noises coming from PLQ densities. Amazingly, it turns out that the IP method used in (Aravkin et al., 2011a) generalizes perfectly to the entire class of PLQ densities under a simple verifiable non-degeneracy condition. In practice, IP methods converge in a small number of iterations, and the effort per iteration depends on the structure of the underlying problem. We show that the IP

iterations for all PLQ Kalman smoothing problems can be computed with a number of operations that scales linearly in  $N$ , as in the quadratic case. This theoretical foundation generalizes the results recently obtained in (Aravkin et al., 2011a,b; Farahmand et al., 2011; Ohlsson et al., 2011), framing them as particular cases of the general framework presented here.

The paper is organized as follows. In Section 2 we introduce the class of QS convex functions, and give sufficient conditions that allow us to interpret these functions as the negative logs of associated probability densities. In Section 3 we show how to construct QS penalties and densities having a desired structure from basic components, and in particular how multivariate densities can be endowed with prescribed means and variances using scalar building blocks. To illustrate this procedure, further details are provided for the Huber and Vapnik penalties. In Section 4, we focus on PLQ penalties, derive the associated KKT system, and present a theorem that guarantees convergence of IP methods under appropriate hypotheses. In Section 5, we present the Kalman smoothing dynamic model, formulate Kalman smoothing with PLQ penalties, present the KKT system for the dynamic case, and show that IP iterations for PLQ smoothing preserve the classical computational efficiency known for the Gaussian case. We present numerical examples using both simulated and real data in Section 6, and make some concluding remarks in Section 7. Section 8 serves as an appendix where supporting mathematical results and proofs are presented.

## 2. Quadratic Support Functions and Densities

In this section, we introduce the class of Quadratic Support (QS) functions, characterize some of their properties, and show that many commonly used penalties fall into this class. We also give a statistical interpretation to QS penalties by interpreting them as negative log likelihoods of probability densities; this relationship allows prescribing means and variances along with the general quality of the error model, an essential requirement of the Kalman smoothing framework and many other areas.

### 2.1 Preliminaries

We recall a few definitions from convex analysis, required to specify the domains of QS penalties. The reader is referred to (Rockafellar, 1970; Rockafellar and Wets, 1998) for more detailed reading.

- (Affine hull) Define the affine hull of any set  $C \subset \mathbb{R}^n$ , denoted by  $\text{aff}(C)$ , as the smallest affine set (translated subspace) that contains  $C$ .
- (Cone) For any set  $C \subset \mathbb{R}^n$ , denote by  $\text{cone } C$  the set  $\{tr | r \in C, t \in \mathbb{R}_+\}$ .
- (Domain) For  $f(x) : \mathbb{R}^n \rightarrow \overline{\mathbb{R}} = \{\mathbb{R} \cup \infty\}$ ,  $\text{dom}(f) = \{x : f(x) < \infty\}$ .
- (Polars of convex sets) For any convex set  $C \subset \mathbb{R}^m$ , the polar of  $C$  is defined to be

$$C^\circ := \{r | \langle r, d \rangle \leq 1 \forall d \in C\},$$

and if  $C$  is a convex cone, this representation is equivalent to

$$C^\circ := \{r | \langle r, d \rangle \leq 0 \forall d \in C\}.$$

- (Horizon cone). Let  $C \subset \mathbb{R}^n$  be a nonempty convex set. The horizon cone  $C^\infty$  is the convex cone of ‘unbounded directions’ for  $C$ , i.e.  $d \in C^\infty$  if  $C + d \subset C$ .

- (Barrier cone). The barrier cone of a convex set  $C$  is denoted by  $\text{bar}(C)$ :

$$\text{bar}(C) := \{x^* | \text{for some } \beta \in \mathbb{R}, \langle x, x^* \rangle \leq \beta \quad \forall x \in C\}.$$

- (Support function). The support function for a set  $C$  is denoted by  $\delta^*(x|C)$ :

$$\delta^*(x|C) := \sup_{c \in C} \langle x, c \rangle.$$

## 2.2 QS functions and densities

We now introduce the QS functions and associated densities that are the focus of this paper. We begin with the dual representation, which is crucial to both establishing a statistical interpretation and to the development of a computational framework.

**Definition 1 (Quadratic Support functions and penalties)** A QS function is any function  $\rho(U, M, b, B; \cdot) : \mathbb{R}^n \rightarrow \mathbb{R}$  having representation

$$\rho(U, M, b, B; y) = \sup_{u \in U} \left\{ \langle u, b + By \rangle - \frac{1}{2} \langle u, Mu \rangle \right\}, \quad (2.1) \text{?PLQpenalty?}$$

where  $U \subset \mathbb{R}^m$  is a nonempty convex set,  $M \in \mathcal{S}_+^n$  the set of real symmetric positive semidefinite matrices, and  $b + By$  is an injective affine transformation in  $y$ , with  $B \in \mathbb{R}^{m \times n}$ , so, in particular,  $m \leq n$  and  $\text{null}(B) = \{0\}$ .

When  $0 \in U$ , we refer to the associated QS function as a penalty, since it is necessarily non-negative.

**Remark 2** When  $U$  is polyhedral,  $0 \in U$ ,  $b = 0$  and  $B = I$ , we recover the basic piecewise linear-quadratic penalties characterized in (Rockafellar and Wets, 1998, Example 11.18).

**Theorem 3** Let  $U, M, B, b$  be as in Definition 1, and set  $K = U^\infty \cap \text{null}(M)$ . Then

$$B^{-1}[\text{bar}(U) + \text{Ran}(M) - b] \subset \text{dom}[\rho(U, M, B, b; \cdot)] \subset B^{-1}[K^\circ - b],$$

with equality throughout when  $\text{bar}(U) + \text{Ran}(M)$  is closed, where  $\text{bar}(U) = \text{dom}(\delta^*(\cdot|U))$  is the barrier cone of  $U$ . In particular, equality always holds when  $U$  is polyhedral.

We now show that many commonly used penalties are special cases of QS (and indeed, of the PLQ) class.

**Remark 4 (scalar examples)**  $\ell_2$ ,  $\ell_1$ , elastic net, Huber, hinge, and Vapnik penalties are all representable using the notation of Definition 1.

1.  $\ell_2$ : Take  $U = \mathbb{R}$ ,  $M = 1$ ,  $b = 0$ , and  $B = 1$ . We obtain

$$\rho(y) = \sup_{u \in \mathbb{R}} \{uy - u^2/2\}.$$

The function inside the sup is maximized at  $u = y$ , hence  $\rho(y) = \frac{1}{2}y^2$ , see top left panel of Fig. 1.

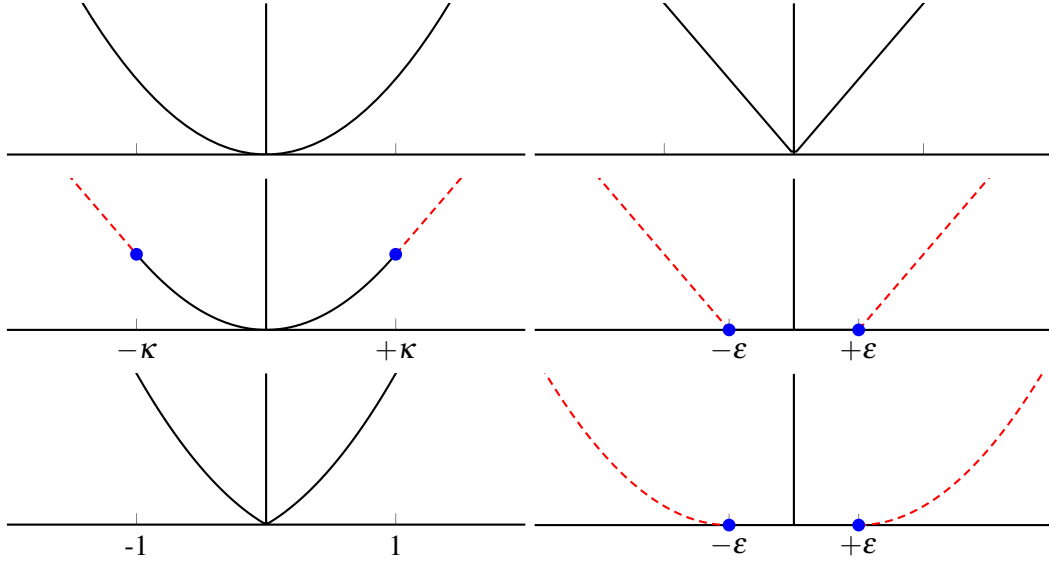


Figure 1: Scalar  $\ell_2$  (top left),  $\ell_1$  (top right), Huber (middle left), Vapnik (middle right), elastic net (bottom left) and smooth insensitive loss (bottom right) penalties

2.  $\ell_1$ : Take  $U = [-1, 1]$ ,  $M = 0$ ,  $b = 0$ , and  $B = 1$ . We obtain

$$\rho(y) = \sup_{u \in [-1, 1]} \{uy\} .$$

The function inside the sup is maximized by taking  $u = \text{sign}(y)$ , hence  $\rho(y) = |y|$ , see top right panel of Fig. 1.

3. Elastic net:  $\ell_2 + \lambda \ell_1$ . Take

$$U = \mathbb{R} \times [-\lambda, \lambda], \quad b = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad M = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad B = \begin{bmatrix} 1 \\ 1 \end{bmatrix} .$$

This construction reveals the general calculus of PLQ addition, see Remark 5. See bottom right panel of Fig. 1.

4. Huber: Take  $U = [-\kappa, \kappa]$ ,  $M = 1$ ,  $b = 0$ , and  $B = 1$ . We obtain

$$\rho(y) = \sup_{u \in [-\kappa, \kappa]} \{uy - u^2/2\} ,$$

with three explicit cases:

- (a) If  $y < -\kappa$ , take  $u = -\kappa$  to obtain  $-\kappa y - \frac{1}{2}\kappa^2$ .
- (b) If  $-\kappa \leq y \leq \kappa$ , take  $u = y$  to obtain  $\frac{1}{2}y^2$ .
- (c) If  $y > \kappa$ , take  $u = \kappa$  to obtain a contribution of  $\kappa y - \frac{1}{2}\kappa^2$ .

This is the Huber penalty, shown in the middle left panel of Fig. 1.

5. Hinge loss: Taking  $B = 1$ ,  $b = -\varepsilon$ ,  $M = 0$  and  $U = [0, 1]$  we have

$$\rho(y) = \sup_{u \in U} \{(y - \varepsilon)u\} = (y - \varepsilon)_+.$$

To verify this, just note that if  $y < \varepsilon$ ,  $u^* = 0$ ; otherwise  $u^* = 1$ .

6. Vapnik loss is given by  $(y - \varepsilon)_+ + (-y - \varepsilon)_+$ . We immediately obtain its PLQ representation by taking

$$B = \begin{bmatrix} 1 \\ -1 \end{bmatrix}, b = -\begin{bmatrix} \varepsilon \\ \varepsilon \end{bmatrix}, M = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}, U = [0, 1] \times [0, 1]$$

to yield

$$\rho(y) = \sup_{u \in U} \left\{ \left\langle \begin{bmatrix} y - \varepsilon \\ -y - \varepsilon \end{bmatrix}, u \right\rangle \right\} = (y - \varepsilon)_+ + (-y - \varepsilon)_+.$$

The Vapnik penalty is shown in the middle right panel of Fig. 1.

7. Soft hinge loss function (Chu et al., 2001). Combining ideas from examples 4 and 5, we can construct a ‘soft’ hinge loss; i.e. the function

$$\rho(y) = \begin{cases} 0 & \text{if } y < \varepsilon \\ \frac{1}{2}(y - \varepsilon)^2 & \text{if } \varepsilon < y < \varepsilon + \kappa \\ \kappa(y - \varepsilon) - \frac{1}{2}(\kappa)^2 & \text{if } \varepsilon + \kappa < y. \end{cases}$$

that has a smooth (quadratic) transition rather than a kink at  $\varepsilon$ : Taking  $B = 1$ ,  $b = -\varepsilon$ ,  $M = 1$  and  $U = [0, \kappa]$  we have

$$\rho(y) = \sup_{u \in [0, \kappa]} \{(y - \varepsilon)u\} - \frac{1}{2}u^2.$$

To verify this function has the explicit representation given above, note that if  $y < \varepsilon$ ,  $u^* = 0$ ; if  $\varepsilon < y < \varepsilon + \kappa$ , we have  $u^* = (y - \varepsilon)_+$ , and if  $\varepsilon + \kappa < y$ , we have  $u^* = \kappa$ .

8. Soft insensitive loss function (Chu et al., 2001). Using example 7, we can create a symmetric soft insensitive loss function (which one might term the Hubnik) by adding together to soft hinge loss functions:

$$\begin{aligned} \rho(y) &= \sup_{u \in [0, \kappa]} \{(y - \varepsilon)u\} - \frac{1}{2}u^2 + \sup_{u \in [0, \kappa]} \{(-y - \varepsilon)u\} - \frac{1}{2}u^2 \\ &= \sup_{u \in [0, \kappa]^2} \left\{ \left\langle \begin{bmatrix} y - \varepsilon \\ -y - \varepsilon \end{bmatrix}, u \right\rangle \right\} - \frac{1}{2}u^T \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} u. \end{aligned}$$

See bottom bottom right panel of Fig. 1.

Note that the affine generalization (Definition 1) is needed to form the elastic net, the Vapnik penalty, and the SILF function, as all of these are sums of simpler QS penalties. These sum constructions are examples of a general calculus which allows the modeler to build up a QS density having a desired structure. This calculus is described in the following remark.

**Remark 5** Let  $\rho_1(y)$  and  $\rho_2(y)$  be two QS penalties specified by  $U_i, M_i, b_i, B_i$ , for  $i = 1, 2$ . Then the sum  $\rho(y) = \rho_1(y) + \rho_2(y)$  is also a QS penalty, with

$$U = U_1 \times U_2, M = \begin{bmatrix} M_1 & 0 \\ 0 & M_2 \end{bmatrix}, b = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}, B = \begin{bmatrix} B_1 \\ B_2 \end{bmatrix}.$$

Notwithstanding the catalogue of scalar QS functions in Remark 4 and the gluing procedure described in Remark 5, the supremum in Definition 1 appears to be a significant roadblock to understanding and designing a QS function having specific properties. However, with some practice the design of QS penalties is not as daunting a task as it first appears. A key tool in understanding the structure of QS functions are Euclidean norm projections onto convex sets.

**Theorem 6 (Projection Theorem for Convex Sets)** [Zarantonello (1971)] Let  $Q \in \mathbb{R}^{n \times n}$  be symmetric and positive definite and let  $C \subset \mathbb{R}^n$  be non-empty, closed and convex. Then  $Q$  defines an inner product on  $\mathbb{R}^n$  by  $\langle x, y \rangle_Q = x^T Q y$  with associated Euclidean norm  $\|x\|_Q = \sqrt{\langle x, x \rangle_Q}$ . The projection of a point  $y \in \mathbb{R}^n$  onto  $C$  in norm  $\|\cdot\|_Q$  is the unique point  $P_Q(y|C)$  solving the least distance problem

$$\inf_{x \in C} \|y - x\|_Q, \quad (2.2) \text{proj\_dist?}$$

and  $z = P_Q(y|C)$  if and only if  $z \in C$  and

$$\langle x - z, y - z \rangle_Q \leq 0 \quad \forall x \in C. \quad (2.3) \text{proj\_oc?}$$

Note that the least distance problem (2.2) is equivalent to the problem

$$\inf_{x \in C} \frac{1}{2} \|y - x\|_Q^2.$$

In the following lemma we use projections as well as duality theory to provide alternative representations for QS penalties.

**Theorem 7** Let  $M \in \mathbb{R}^{n \times n}$  be symmetric and positive semi-definite matrix, let  $L \in \mathbb{R}^{n \times k}$  be any matrix satisfying  $M = LL^T$  where  $k = \text{rank}(M)$ , and let  $U \subset \mathbb{R}^n$  be a non-empty, closed and convex set that contains the origin. Then the QS function  $\rho := \rho(U, M, 0, I; \cdot)$  has the primal representations

$$\rho(y) = \inf_{s \in \mathbb{R}^k} \left[ \frac{1}{2} \|s\|_2^2 + \delta^*(y - Ls | U) \right] = \inf_{s \in \mathbb{R}^k} \left[ \frac{1}{2} \|s\|_2^2 + \gamma(y - Ls | U^\circ) \right], \quad (2.4) \text{QS\_primal?}$$

where, for any convex set  $V$ ,

$$\delta^*(z|V) := \sup_{v \in V} \langle z, v \rangle \quad \text{and} \quad \gamma(z|V) := \inf \{t \mid t \geq 0, z \in tV\}$$

are the support and gauge functionals for  $V$ , respectively.

If it is further assumed that  $M \in \mathcal{S}_{++}^n$  the set of positive definite matrices, then  $\rho$  has the represen-



tations

$$\rho(y) = \inf_{s \in \mathbb{R}^k} \left[ \frac{1}{2} \|s\|_M^2 + \gamma(M^{-1}y - s | M^{-1}U^\circ) \right] \quad (2.5) \{?\}$$

$$= \frac{1}{2} \|P_M(M^{-1}y | U)\|_M^2 + \gamma(M^{-1}y - P_M(M^{-1}y | U) | M^{-1}U^\circ) \quad (2.6) \{?\}$$

$$= \inf_{s \in \mathbb{R}^k} \left[ \frac{1}{2} \|s\|_{M^{-1}}^2 + \gamma(y - s | U^\circ) \right] \quad (2.7) \{?\}$$

$$= \frac{1}{2} \|P_{M^{-1}}(y | MU)\|_{M^{-1}}^2 + \gamma(y - P_{M^{-1}}(y | MU) | U^\circ) \quad (2.8) \{?\}$$

$$= \frac{1}{2} y^T M^{-1} y - \inf_{u \in MU} \frac{1}{2} \|u - M^{-1}y\|_M^2 \quad (2.9) \{?\}$$

$$= \frac{1}{2} \|P_M(M^{-1}y | U)\|_M^2 + \langle M^{-1}y - P_M(M^{-1}y | U), P_M(M^{-1}y | U) \rangle_M \quad (2.10) \{?\}$$

$$= \frac{1}{2} y^T M^{-1} y - \inf_{v \in MU} \frac{1}{2} \|v - y\|_{M^{-1}}^2 \quad (2.11) \{?\}$$

$$= \frac{1}{2} \|P_{M^{-1}}(y | MU)\|_{M^{-1}}^2 + \langle y - P_{M^{-1}}(y | MU), P_{M^{-1}}(y | MU) \rangle_{M^{-1}} . \quad (2.12) \{?\}$$

In particular, (2.11) says  $\rho(y) = \frac{1}{2} y^T M^{-1} y$  whenever  $y \in MU$ . Also note that, by (2.4), one can replace the gauge functionals in (2.5)-(2.8) by the support functional of the appropriate set where  $M^{-1}U^\circ = (MU)^\circ$ .

The formulas (2.5)-(2.12) show how one can build PLQ penalties having a wide range of desirable properties. We now give a short list of a few examples illustrating how to make use of these representations.

**Remark 8 (General examples)** In this remark we show how the representations in Lemma 7 can be used to build QS penalties with specific structure. In each example we specify the components  $U, M, b$ , and  $B$  for the QS function  $\rho := \rho(U, M, b, B; \cdot)$ .

1. *Norms.* Any norm  $\|\cdot\|$  can be represented as a QS function by taking  $M = 0, B = I, b = 0, U = \mathbb{B}^\circ$ , where  $\mathbb{B}$  is the unit ball of the desired norm. Then, by (2.4),  $\rho(y) = \|y\| = \gamma(y | \mathbb{B})$ .
2. *Gauges and support functions.* Let  $U$  be any closed convex set containing the origin, and Take  $M = 0, B = I, b = 0$ . Then, by (2.4),  $\rho(y) = \gamma(y | U^\circ) = \delta^*(y | U)$ .
3. *Generalized Huber functions.* Take any norm  $\|\cdot\|$  having closed unit ball  $\mathbb{B}$ . Let  $M \in \mathcal{S}_{++}^n, B = I, b = 0$ , and  $U = \mathbb{B}^\circ$ . Then, by the representation (2.8),

$$\rho(y) = \frac{1}{2} P_{M^{-1}}(y | M\mathbb{B}^\circ)^T M^{-1} P_{M^{-1}}(y | M\mathbb{B}^\circ) + \|y - P_{M^{-1}}(y | M\mathbb{B}^\circ)\| . \quad (2.13) \text{?g-Huber?}$$

In particular, for  $y \in M\mathbb{B}^\circ$ ,  $\rho(y) = \frac{1}{2} y^T M^{-1} y$ .

If we take  $M = I$  and  $\|\cdot\| = \kappa^{-1} \|\cdot\|_1$  for  $\kappa > 0$  (i.e.  $U = \kappa \mathbb{B}_\infty$  and  $U^\circ = \kappa^{-1} \mathbb{B}_1$ ), then  $\rho$  is the multivariate Huber function described in item 4 of Remark 4. In this way, Theorem 7 shows how to generalize the essence of the Huber norm to any choice of norm. For example, if we take  $U = \kappa \mathbb{B}_M = \{\kappa u \mid \|u\|_M \leq 1\}$ , then, by (2.10),

$$\rho(y) = \begin{cases} \frac{1}{2} \|y\|_{M^{-1}}^2 & , \text{if } \|y\|_{M^{-1}} \leq \kappa \\ \kappa \|y\|_{M^{-1}} - \frac{\kappa^2}{2} & , \text{if } \|y\|_{M^{-1}} > \kappa . \end{cases}$$

4. *Generalized hinge-loss functions.* Let  $\|\cdot\|$  be a norm with closed unit ball  $\mathbb{B}$ , let  $K$  be a non-empty closed convex cone in  $\mathbb{R}^n$ , and let  $v \in \mathbb{R}^n$ . Set  $M = 0$ ,  $b = -v$ ,  $B = I$ , and  $U = -(\mathbb{B}^\circ \cap K^\circ) = \mathbb{B}^\circ \cap (-K)^\circ$ . Then, by (Burke, 1987, Section 2),

$$\rho(y) = \text{dist}(y | v - K) = \inf_{u \in K} \|y - b + u\|.$$

If we consider the order structure “ $\leq_K$ ” induced on  $\mathbb{R}^n$  by

$$y \leq_K v \iff v - y \in K,$$

then  $\rho(y) = 0$  if and only if  $y \leq_K v$ . By taking  $\|\cdot\| = \|\cdot\|_1$ ,  $K = \mathbb{R}_+^n$  so  $(-K)^\circ = K$ , and  $v = \varepsilon \mathbf{1}$ , where  $\mathbf{1}$  is the vector of all ones, we recover the multivariate hinge loss function in Remark 4.

5. *Order intervals and Vapnik loss functions.* Let  $\|\cdot\|$  be a norm with closed unit ball  $\mathbb{B}$ , let  $K \subset \mathbb{R}^n$  be a non-empty symmetric convex cone in the sense that  $K^\circ = -K$ , and let  $w <_K v$ , or equivalently,  $v - w \in \text{intr}(K)$ . Set

$$U = (\mathbb{B}^\circ \cap K) \times (\mathbb{B}^\circ \cap K^\circ), \quad M = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}, \quad b = -\begin{pmatrix} v \\ w \end{pmatrix}, \quad \text{and} \quad B = \begin{bmatrix} I \\ I \end{bmatrix}.$$

Then

$$\rho(y) = \text{dist}(y | v - K) + \text{dist}(y | w + K).$$

Observe that  $\rho(y) = 0$  if and only if  $w \leq_K y \leq_K v$ . The set  $\{y | w \leq_K y \leq_K v\}$  is an “order interval” (Schaefer, 1970). If we take  $w = -v$ , then  $\{y | -v \leq_K y \leq_K v\}$  is a symmetric neighborhood of the origin. By taking  $\|\cdot\| = \|\cdot\|_1$ ,  $K = \mathbb{R}_+^n$ , and  $v = \varepsilon \mathbf{1} = -w$ , we recover the multivariate Vapnik loss function in Remark 4. Further examples of symmetric cones are  $\mathcal{S}_+^n$  and the Lorentz or  $\ell_2$  cone (Güler and Hauser, 2002).

The examples given above show that one can also construct generalized versions of the elastic net as well as the soft insensitive loss functions defined in Remark 4. In addition, cone constraints can also be added by using the identity  $\delta^*(\cdot | K^\circ) = \delta(\cdot | K)$ . These examples serve to illustrate the wide variety of penalty functions representable as QS functions. Computationally, one is only limited by the ability to compute projections described in Theorem 7. Further computational properties for QS functions are described in (Aravkin et al., 2012, Section 6).

In order to characterize QS functions as negative logs of density functions, we need to ensure the integrability of said density functions. The function  $\rho(y)$  is said to be *coercive* if  $\lim_{\|y\| \rightarrow \infty} \rho(y) = \infty$ , and coercivity turns out to be the key property to ensure integrability. The proof of this fact and the characterization of coercivity for QS functions are the subject of the next two theorems (see Appendix for proofs).

**Theorem 9 (QS integrability)** Suppose  $\rho(y)$  is a coercive QS penalty. Then the function  $\exp[-\rho(y)]$  is integrable on  $\text{aff}[\text{dom}(\rho)]$  with respect to the  $\dim(\text{aff}[\text{dom}(\rho)])$ -dimensional Lebesgue measure.

**Theorem 10** A QS function  $\rho$  is coercive if and only if  $[B^T \text{cone}(U)]^\circ = \{0\}$ .

Theorem 10 can be used to show the coercivity of familiar penalties. In particular, note that if  $B = I$ , then the QS function is coercive if and only if  $U$  contains the origin in its interior.

**Corollary 11** *The penalties  $\ell_2$ ,  $\ell_1$ , elastic net, Vapnik, and Huber are all coercive.*

**Proof** We show that all of these penalties satisfy the hypothesis of Theorem 10.

$\ell_2$ :  $U = \mathbb{R}$  and  $B = 1$ , so  $[B^T \text{cone}(U)]^\circ = \mathbb{R}^\circ = \{0\}$ .

$\ell_1$ :  $U = [-1, 1]$ , so  $\text{cone}(U) = \mathbb{R}$ , and  $B = 1$ .

Elastic Net: In this case,  $\text{cone}(U) = \mathbb{R}^2$  and  $B = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ .

Huber:  $U = [-\kappa, \kappa]$ , so  $\text{cone}(U) = \mathbb{R}$ , and  $B = 1$ .

Vapnik:  $U = [0, 1] \times [0, 1]$ , so  $\text{cone}(U) = \mathbb{R}_+^2$ .  $B = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$ , so  $B^T \text{cone}(U) = \mathbb{R}$ .

■

One can also show the coercivity of the above examples using their primal representations. However, our main objective is to pave the way for a modeling framework where multi-dimensional penalties can be constructed from simple building blocks and then solved by a uniform approach, using the dual representations alone.

We now define a family of distributions on  $\mathbb{R}^n$  by interpreting piecewise linear quadratic functions  $\rho$  as negative logs of corresponding densities. Note that the support of the distributions is always contained in  $\text{dom } \rho$ , characterized, in Theorem 3.

**Definition 12 (QS densities)** *Let  $\rho(U, M, B, b; y)$  be any coercive extended QS penalty on  $\mathbb{R}^n$ . Define  $\mathbf{p}(y)$  to be the following density on  $\mathbb{R}^n$ :*

$$\mathbf{p}(y) = \begin{cases} c^{-1} \exp[-\rho(y)] & y \in \text{dom } \rho \\ 0 & \text{else,} \end{cases} \quad (2.14) \text{ ?PLQdensity?}$$

where

$$c = \left( \int_{y \in \text{dom } \rho} \exp[-\rho(y)] dy \right),$$

and the integral is with respect to the  $\dim(\text{dom}(\rho))$ -dimensional Lebesgue measure.

QS densities are true densities on the affine hull of the domain of  $\rho$ . The proof of Theorem 9 can be easily adapted to show that they have moments of all orders.

### 3. Constructing QS densities

In this section, we describe how to construct multivariate QS densities with prescribed means and variances. We show how to compute normalization constants to obtain scalar densities, and then extend to multivariate densities using linear transformations. Finally, we show how to obtain the data structures  $U, M, B, b$  corresponding to multivariate densities, since these are used by the optimization approach in Section 4.

We make use of the following definitions. Given a sequence of column vectors  $\{r_k\} = \{r_1, \dots, r_N\}$  and matrices  $\{\Sigma_k\} = \{\Sigma_1, \dots, \Sigma_N\}$ , we use the notation

$$\text{vec}(\{r_k\}) = \begin{bmatrix} r_1 \\ r_2 \\ \vdots \\ r_N \end{bmatrix}, \quad \text{diag}(\{\Sigma_k\}) = \begin{bmatrix} \Sigma_1 & 0 & \cdots & 0 \\ 0 & \Sigma_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \Sigma_N \end{bmatrix}.$$

In definition 12, QS densities are defined over  $\mathbb{R}^n$ . The moments of these densities depend in a nontrivial way on the choice of parameters  $b, B, U, M$ . In practice, we would like to be able to construct these densities to have prescribed means and variances. We now show how this can be done using scalar QS random variables as the building blocks. Suppose  $y = \text{vec}(\{y_k\})$  is a vector of independent (but not necessarily identical) QS random variables with mean 0 and variance 1. Denote by  $b_k, B_k, U_k, M_k$  the specification for the densities of  $y_k$ . To obtain the density of  $y$ , we need only take

$$\begin{aligned} U &= U_1 \times U_2 \times \cdots \times U_N \\ M &= \text{diag}(\{M_k\}) \\ B &= \text{diag}(\{B_k\}) \\ b &= \text{vec}(\{b_k\}) . \end{aligned}$$

For example, the standard Gaussian distribution is specified by  $U = \mathbb{R}^n$ ,  $M = I$ ,  $b = 0$ ,  $B = I$ , while the standard  $\ell_1$ -Laplace (see (Aravkin et al., 2011a)) is specified by  $U = [-1, 1]^n$ ,  $M = 0$ ,  $b = 0$ ,  $B = \sqrt{2}I$ .

The random vector  $\tilde{y} = Q^{1/2}(y + \mu)$  has mean  $\mu$  and variance  $Q$ . If  $c$  is the normalizing constant for the density of  $y$ , then  $c \det(Q)^{1/2}$  is the normalizing constant for the density of  $\tilde{y}$ .

**Remark 13** *Note that only independence of the building blocks is required in the above result. This allows the flexibility to impose different QS densities on different errors in the model. Such flexibility may be useful for example when combining measurement data from different instruments, where some instruments may occasionally give bad data (with outliers), while others have errors that are modeled well by Gaussian distributions.*

We now show how to construct scalar building blocks with mean 0 and variance 1, i.e. how to compute the key normalizing constants for any QS penalty. To this aim, suppose  $\rho(y)$  is a scalar QS penalty that is symmetric about 0. We would like to construct a density  $\mathbf{p}(y) = \exp[-\rho(c_2 y)] / c_1$  to be a true density with unit variance, that is,

$$\frac{1}{c_1} \int \exp[-\rho(c_2 y)] dy = 1 \quad \text{and} \quad \frac{1}{c_1} \int y^2 \exp[-\rho(c_2 y)] dy = 1, \quad (3.1) \text{?PLQconst?}$$

where the integrals are over  $\mathbb{R}$ . Using  $u$ -substitution, these equations become

$$c_1 c_2 = \int \exp[-\rho(y)] dy \quad \text{and} \quad c_1 c_2^3 = \int y^2 \exp[-\rho(y)] dy.$$

Solving this system yields

$$\begin{aligned} c_2 &= \sqrt{\int y^2 \exp[-\rho(y)] dy / \int \exp[-\rho(y)] dy} \\ c_1 &= \frac{1}{c_2} \int \exp[-\rho(y)] dy . \end{aligned}$$

These expressions can be used to obtain the normalizing constants for any particular  $\rho$  using simple integrals.

### 3.1 Huber Density

The scalar density corresponding to the Huber penalty is constructed as follows. Set

$$\mathbf{p}_H(y) = \frac{1}{c_1} \exp[-\rho_H(c_2 y)], \quad (3.2) \text{HuberDensityScalar}$$

where  $c_1$  and  $c_2$  are chosen as in (3.1). Specifically, we compute

$$\begin{aligned} \int \exp[-\rho_H(y)] dy &= 2 \exp[-\kappa^2/2] \frac{1}{\kappa} + \sqrt{2\pi}[2\Phi(\kappa) - 1] \\ \int y^2 \exp[-\rho_H(y)] dy &= 4 \exp[-\kappa^2/2] \frac{1+\kappa^2}{\kappa^3} + \sqrt{2\pi}[2\Phi(\kappa) - 1], \end{aligned}$$

where  $\Phi$  is the standard normal cumulative density function. The constants  $c_1$  and  $c_2$  can now be readily computed.

To obtain the multivariate Huber density with variance  $Q$  and mean  $\mu$ , let  $U = [-\kappa, \kappa]^n$ ,  $M = I$ ,  $B = I$  any full rank matrix, and  $b = 0$ . This gives the desired density:

$$\mathbf{p}_H(y) = \frac{1}{c_1^n \det(Q^{1/2})} \exp \left[ - \sup_{u \in U} \left\{ \left\langle c_2 Q^{-1/2} (y - \mu), u \right\rangle - \frac{1}{2} u^T u \right\} \right]. \quad (3.3) \text{HuberDensity}$$

### 3.2 Vapnik Density

The scalar density associated with the Vapnik penalty is constructed as follows. Set

$$\mathbf{p}_V(y) = \frac{1}{c_1} \exp[-\rho_V(c_2 y)], \quad (3.4) \text{VapnikDensityScalar}$$

where the normalizing constants  $c_1$  and  $c_2$  can be obtained from

$$\begin{aligned} \int \exp[-\rho_V(y)] dy &= 2(\varepsilon + 1) \\ \int y^2 \exp[-\rho_V(y)] dy &= \frac{2}{3} \varepsilon^3 + 2(2 - 2\varepsilon + \varepsilon^2), \end{aligned}$$

using the results in Section 3. Taking  $U = [0, 1]^{2n}$ , the multivariate Vapnik distribution with mean  $\mu$  and variance  $Q$  is

$$\mathbf{p}_V(y) = \frac{1}{c_1^n \det(Q^{1/2})} \exp \left[ - \sup_{u \in U} \left\{ \left\langle c_2 B Q^{-1/2} (y - \mu) - \varepsilon \mathbf{1}_{2n}, u \right\rangle \right\} \right], \quad (3.5) \text{VapnikDensity}$$

where  $B$  is block diagonal with each block of the form  $B = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$ , and  $\mathbf{1}_{2n}$  is a column vector of 1's of length  $2n$ .

## 4. Optimization with PLQ penalties

In the previous sections, QS penalties were characterized using their dual representation and interpreted as negative log likelihoods of true densities. As we have seen, the scope of such densities is extremely broad. Moreover, these densities can easily be constructed to possess specified moment

properties. In this section, we expand on their utility by showing that the resulting estimation problems (1.4) can be solved with high accuracy using standard techniques from numerical optimization for a large subclass of these penalties. We focus on PLQ penalties for the sake of simplicity in our presentation of an interior point approach to solving these estimation problems. However, the interior point approach applies in much more general settings, e.g. see Nemirovskii and Nesterov (1994). Nonetheless, the PLQ case is sufficient to cover all of the examples given in Remark 4 while giving the flavor of how to proceed in the more general cases.

We exploit the dual representation for the class of PLQ penalties (Rockafellar and Wets, 1998) to explicitly construct the Karush-Kuhn-Tucker (KKT) conditions for a wide variety of model problems of the form (1.4). Working with these systems opens the door to using a wide variety of numerical methods for convex quadratic programming to solve (1.4).

Let  $\rho(U_v, M_v, b_v, B_v; y)$  and  $\rho(U_w, M_w, b_w, B_w; y)$  be two PLQ penalties and define

$$V(v; R) := \rho(U_v, M_v, b_v, B_v; R^{-1/2}v) \quad (4.1) \text{?PLQ-V?}$$

and

$$W(w; Q) := \rho(U_w, M_w, b_w, B_w; Q^{-1/2}w). \quad (4.2) \text{?PLQ-W?}$$

Then (1.4) becomes

$$\min_{y \in \mathbb{R}^n} \rho(U, M, b, B; y), \quad (4.3) \text{?newopt?}$$

where

$$U := U_v \times U_w, \quad M := \begin{bmatrix} M_v & 0 \\ 0 & M_w \end{bmatrix}, \quad b := \begin{pmatrix} b_v - B_v R^{-1/2} z \\ b_w - B_w Q^{-1/2} \mu \end{pmatrix},$$

and

$$B := \begin{bmatrix} B_v R^{-1/2} H \\ B_w Q^{-1/2} G \end{bmatrix}.$$

Moreover, the hypotheses in (1.1), (1.2), (1.4), and (2.1) imply that the matrix  $B$  in (4.3) is injective. Indeed,  $By = 0$  if and only if  $B_w Q^{-1/2} G y = 0$ , but, since  $G$  is nonsingular and  $B_w$  is injective, this implies that  $y = 0$ . That is,  $\text{nul}(B) = \{0\}$ . Consequently, the objective in (4.3) takes the form of a PLQ penalty function (2.1). In particular, if (4.1) and (4.2) arise from PLQ densities (definition 12), then the solution to problem (4.3) is the MAP estimator in the statistical model (1.1)-(1.2).

To simplify the notational burden, in the remainder of this section we work with (4.3) directly and assume that the defining objects in (4.3) have the dimensions specified in (2.1);

$$U \in \mathbb{R}^m, \quad M \in \mathbb{R}^{m \times m}, \quad b \in \mathbb{R}^m, \quad \text{and} \quad B \in \mathbb{R}^{m \times n}. \quad (4.4) \text{?PLQdimSpecs?}$$

The Lagrangian (Rockafellar and Wets, 1998)[Example 11.47] for problem (4.3) is given by

$$L(y, u) = b^T u - \frac{1}{2} u^T M u + u^T B y.$$

By assumption  $U$  is polyhedral, and so can be specified to take the form

$$U = \{u : A^T u \leq a\}, \quad (4.5) \text{?polyhedralU?}$$

where  $A \in \mathbb{R}^{m \times \ell}$ . Using this representation for  $U$ , the optimality conditions for (4.3) (Rockafellar, 1970; Rockafellar and Wets, 1998) are

$$\begin{aligned} 0 &= B^T u \\ 0 &= b + By - Mu - Aq \\ 0 &= A^T u + s - a \\ 0 &= q_i s_i, \quad i = 1, \dots, \ell, \quad q, s \geq 0, \end{aligned} \tag{4.6} \text{?fullKKT?}$$

where the non-negative slack variable  $s$  is defined by the third equation in (4.6). The non-negativity of  $s$  implies that  $u \in U$ . The equations  $0 = q_i s_i$ ,  $i = 1, \dots, \ell$  in (4.6) are known as the complementarity conditions. By convexity, solving the problem (4.3) is equivalent to satisfying (4.6). There is a vast optimization literature on working directly with the KKT system. In particular, interior point (IP) methods (Kojima et al., 1991; Nemirovskii and Nesterov, 1994; Wright, 1997) can be employed. In the Kalman filtering/smoothing application, IP methods have been used to solve the KKT system (4.6) in a numerically stable and efficient manner, see e.g. (Aravkin et al., 2011b). Remarkably, the IP approach used in (Aravkin et al., 2011b) generalizes to the entire PLQ class. For Kalman filtering and smoothing, the computational efficiency is also preserved (see Section 5). Here, we show the general development for the entire PLQ class using standard techniques from the IP literature.

Let  $U, M, b, B$ , and  $A$  be as defined in (2.1) and (4.5), and let  $\tau \in (0, +\infty]$ . We define the  $\tau$  *slice of the strict feasibility region* for (4.6) to be the set

$$\mathcal{F}_+(\tau) = \left\{ (s, q, u, y) \mid \begin{array}{l} 0 < s, \quad 0 < q, \quad s^T q \leq \tau, \text{ and} \\ (s, q, u, y) \text{ satisfy the affine equations in (4.6)} \end{array} \right\},$$

and the *central path* for (4.6) to be the set

$$\mathcal{C} := \left\{ (s, q, u, y) \mid \begin{array}{l} 0 < s, \quad 0 < q, \quad \gamma = q_i s_i \quad i = 1, \dots, \ell, \text{ and} \\ (s, q, u, y) \text{ satisfy the affine equations in (4.6)} \end{array} \right\}.$$

For simplicity, we define  $\mathcal{F}_+ := \mathcal{F}_+(+\infty)$ . The basic strategy of a primal-dual IP method is to follow the central path to a solution of (4.6) as  $\gamma \downarrow 0$  by applying a predictor-corrector damped Newton method to the function mapping  $\mathbb{R}^\ell \times \mathbb{R}^\ell \times \mathbb{R}^m \times \mathbb{R}^n$  to itself given by

$$F_\gamma(s, q, u, y) = \begin{bmatrix} s + A^T u - a \\ D(q)D(s)\mathbf{1} - \gamma\mathbf{1} \\ By - Mu - Aq + b \\ B^T u \end{bmatrix}, \tag{4.7} \text{?rKKT?}$$

where  $D(q)$  and  $D(s)$  are diagonal matrices with vectors  $q, s$  on the diagonal.

**Theorem 14** *Let  $U, M, b, B$ , and  $A$  be as defined in (2.1) and (4.5). Given  $\tau > 0$ , let  $\mathcal{F}_+$ ,  $\mathcal{F}_+(\tau)$ , and  $\mathcal{C}$  be as defined above. If*

$$\mathcal{F}_+ \neq \emptyset \quad \text{and} \quad \text{null}(M) \cap \text{null}(A^T) = \{0\}, \tag{4.8} \text{?key IP?}$$

*then the following statements hold.*

- (i)  $F_\gamma^{(1)}(s, q, u, y)$  is invertible for all  $(s, q, u, y) \in \mathcal{F}_+$ .
- (ii) Define  $\widehat{\mathcal{F}}_+ = \{(s, q) \mid \exists (u, y) \in \mathbb{R}^m \times \mathbb{R}^n \text{ s.t. } (s, q, u, y) \in \mathcal{F}_+\}$ . Then for each  $(s, q) \in \widehat{\mathcal{F}}_+$  there exists a unique  $(u, y) \in \mathbb{R}^m \times \mathbb{R}^n$  such that  $(s, q, u, y) \in \mathcal{F}_+$ .
- (iii) The set  $\mathcal{F}_+(\tau)$  is bounded for every  $\tau > 0$ .
- (iv) For every  $g \in \mathbb{R}_{++}^\ell$ , there is a unique  $(s, q, u, y) \in \mathcal{F}_+$  such that  $g = (s_1 q_1, s_2 q_2, \dots, s_\ell q_\ell)^\top$ .
- (v) For every  $\gamma > 0$ , there is a unique solution  $[s(\gamma), q(\gamma), u(\gamma), y(\gamma)]$  to the equation  $F_\gamma(s, q, u, y) = 0$ . Moreover, these points form a differentiable trajectory in  $\mathbb{R}^v \times \mathbb{R}^v \times \mathbb{R}^m \times \mathbb{R}^n$ . In particular, we may write
$$\mathcal{C} = \{[s(\gamma), q(\gamma), u(\gamma), y(\gamma)] \mid \gamma > 0\}.$$
- (vi) The set of cluster points of the central path as  $\gamma \downarrow 0$  is non-empty, and every such cluster point is a solution to (4.6).

Please see the Appendix for proof. Theorem 14 shows that if the conditions (4.8) hold, then IP techniques can be applied to solve the problem (4.3). In all of the applications we consider, the condition  $\text{null}(M) \cap \text{null}(A^\top) = \{0\}$  is easily verified. For example, in the setting of (4.3) with

$$U_v = \{u \mid A_v u \leq a_v\} \quad \text{and} \quad U_w = \{u \mid A_w u \leq b_w\} \quad (4.9) \text{?}\underline{U_v U_w}?$$

this condition reduces to

$$\text{null}(M_v) \cap \text{null}(A_v^\top) = \{0\} \quad \text{and} \quad \text{null}(M_w) \cap \text{null}(A_w^\top) = \{0\}. \quad (4.10) \text{?}\underline{\text{NullProperty}}?$$

**Corollary 15** *The densities corresponding to  $\ell_1, \ell_2$ , Huber, and Vapnik penalties all satisfy hypothesis (4.10).*

**Proof** We verify that  $\text{null}(M) \cap \text{null}(A^\top) = \{0\}$  for each of the four penalties. In the  $\ell_2$  case,  $M$  has full rank. For the  $\ell_1$ , Huber, and Vapnik penalties, the respective sets  $U$  are bounded, so  $U^\infty = \{0\}$ . ■

On the other hand, the condition  $\mathcal{F}_+ \neq \emptyset$  is typically more difficult to verify. We show how this is done for two sample cases from class (1.4), where the non-emptiness of  $\mathcal{F}_+$  is established by constructing an element of this set. Such constructed points are useful for initializing the interior point algorithm.

#### 4.1 $\ell_1 - \ell_2$ :

Suppose  $V(v; R) = \|R^{-1/2}v\|_1$  and  $W(w; Q) = \frac{1}{2} \|Q^{-1/2}w\|_2^2$ . In this case

$$U_v = [-\mathbf{1}_m, \mathbf{1}_m], \quad M_v = 0_{m \times m}, \quad b_v = 0_m, \quad B_v = I_{m \times m}, \\ U_w = \mathbb{R}^n, \quad M_w = I_{n \times n}, \quad b_w = 0_n, \quad B_w = I_{n \times n},$$



and  $R \in \mathbb{R}^{m \times m}$  and  $Q \in \mathbb{R}^{n \times n}$  are symmetric positive definite covariance matrices. Following the notation of (4.3) we have

$$U = [-\mathbf{1}, \mathbf{1}] \times \mathbb{R}^n, M = \begin{bmatrix} 0_{m \times m} & 0 \\ 0 & I_{n \times n} \end{bmatrix}, b = \begin{pmatrix} -R^{-1/2}z \\ -Q^{-1/2}\mu \end{pmatrix}, B = \begin{bmatrix} R^{-1/2}H \\ Q^{-1/2}G \end{bmatrix}.$$

The specification of  $U$  in (4.5) is given by

$$A^T = \begin{bmatrix} I_{m \times m} & 0_{n \times n} \\ -I_{m \times m} & 0_{n \times n} \end{bmatrix} \text{ and } a = \begin{pmatrix} \mathbf{1} \\ -\mathbf{1} \end{pmatrix}.$$

Clearly, the condition  $\text{null}(M) \cap \text{null}(A^T) = \{0\}$  in (4.8) is satisfied. Hence, for Theorem 14 to apply, we need only check that  $\mathcal{F}_+ \neq \emptyset$ . This is easily established by noting that  $(s, q, u, y) \in \mathcal{F}_+$ , where

$$u = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, y = G^{-1}\mu, s = \begin{pmatrix} \mathbf{1} \\ \mathbf{1} \end{pmatrix}, q = \begin{pmatrix} \mathbf{1} + [R^{-1/2}(Hy - z)]_+ \\ \mathbf{1} - [R^{-1/2}(Hy - z)]_- \end{pmatrix},$$

where, for  $g \in \mathbb{R}^\ell$ ,  $g_+$  is defined componentwise by  $g_{+(i)} = \max\{g_i, 0\}$  and  $g_{-(i)} = \min\{g_i, 0\}$ .

## 4.2 Vapnik – Huber:

Suppose that  $V(v; R)$  and  $W(w; Q)$  are as in (4.1) and (4.2), respectively, with  $V$  a Vapnik penalty and  $W$  a Huber penalty:

$$U_v = [0, \mathbf{1}_m] \times [0, \mathbf{1}_m], M_v = 0_{2m \times 2m}, b_v = -\begin{pmatrix} \varepsilon \mathbf{1}_m \\ \varepsilon \mathbf{1}_m \end{pmatrix}, B_v = \begin{bmatrix} I_{m \times m} \\ -I_{m \times m} \end{bmatrix} \\ U_w = [-\kappa \mathbf{1}_n, \kappa \mathbf{1}_n], M_w = I_{n \times n}, b_w = 0_n, B_w = I_{n \times n},$$

and  $R \in \mathbb{R}^{m \times m}$  and  $Q \in \mathbb{R}^{n \times n}$  are symmetric positive definite covariance matrices. Following the notation of (4.3) we have

$$U = ([0, \mathbf{1}_m] \times [0, \mathbf{1}_m]) \times [-\kappa \mathbf{1}_n, \kappa \mathbf{1}_n], M = \begin{bmatrix} 0_{2m \times 2m} & 0 \\ 0 & I_{n \times n} \end{bmatrix}, \\ b = -\begin{pmatrix} \varepsilon \mathbf{1}_m + R^{-1/2}z \\ \varepsilon \mathbf{1}_m - R^{-1/2}z \\ Q^{-1/2}\mu \end{pmatrix}, B = \begin{bmatrix} R^{-1/2}H \\ -R^{-1/2}H \\ Q^{-1/2}G \end{bmatrix}.$$

The specification of  $U$  in (4.5) is given by

$$A^T = \begin{bmatrix} I_{m \times m} & 0 & 0 \\ -I_{m \times m} & 0 & 0 \\ 0 & I_{m \times m} & 0 \\ 0 & -I_{m \times m} & 0 \\ 0 & 0 & I_{n \times n} \\ 0 & 0 & -I_{n \times n} \end{bmatrix} \text{ and } a = \begin{pmatrix} \mathbf{1}_m \\ 0_m \\ \mathbf{1}_m \\ 0_m \\ \kappa \mathbf{1}_n \\ \kappa \mathbf{1}_n \end{pmatrix}.$$

Since  $\text{null}(A^T) = \{0\}$ , the condition  $\text{null}(M) \cap \text{null}(A^T) = \{0\}$  in (4.8) is satisfied. Hence, for Theorem 14 to apply, we need only check that  $\mathcal{F}_+ \neq \emptyset$ . We establish this by constructing an

element  $(s, q, u, y)$  of  $\mathcal{F}_+$ . For this, let

$$u = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}, s = \begin{pmatrix} s_1 \\ s_2 \\ s_3 \\ s_4 \\ s_5 \\ s_6 \end{pmatrix}, q = \begin{pmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \\ q_5 \\ q_6 \end{pmatrix},$$

and set

$$y = 0_n, u_1 = u_2 = \frac{1}{2}\mathbf{1}_\ell, u_3 = 0_n, s_1 = s_2 = s_3 = s_4 = \frac{1}{2}\mathbf{1}_\ell, s_5 = s_6 = \kappa\mathbf{1}_n,$$

and

$$\begin{aligned} q_1 &= \mathbf{1}_m - (\varepsilon\mathbf{1}_m + R^{-1/2}z)_-, q_2 = \mathbf{1}_m + (\varepsilon\mathbf{1}_m + R^{-1/2}z)_+, \\ q_3 &= \mathbf{1}_m - (\varepsilon\mathbf{1}_m - R^{-1/2}z)_-, q_4 = \mathbf{1}_m + (\varepsilon\mathbf{1}_m - R^{-1/2}z)_+, \\ q_5 &= \mathbf{1}_n - (Q^{-1/2}\mu)_-, q_6 = \mathbf{1}_n + (Q^{-1/2}\mu)_+. \end{aligned}$$

Then  $(s, q, u, y) \in \mathcal{F}_+$ .

## 5. Kalman Smoothing with PLQ penalties

Consider now a dynamic scenario, where the system state  $x_k$  evolves according to the following stochastic discrete-time linear model

$$\begin{aligned} x_1 &= x_0 + w_1 \\ x_k &= G_k x_{k-1} + w_k, \quad k = 2, 3, \dots, N \\ z_k &= H_k x_k + v_k, \quad k = 1, 2, \dots, N \end{aligned} \tag{5.1} \text{?LinearGaussModel}$$

where  $x_0$  is known,  $z_k$  is the  $m$ -dimensional subvector of  $z$  containing the noisy output samples collected at instant  $k$ ,  $G_k$  and  $H_k$  are known matrices. Further, we consider the general case where  $\{w_k\}$  and  $\{v_k\}$  are mutually independent zero-mean random variables which can come from any of the densities introduced in the previous section, with positive definite covariance matrices denoted by  $\{Q_k\}$  and  $\{R_k\}$ , respectively.

In order to formulate the Kalman smoothing problem over the entire sequence  $\{x_k\}$ , define

$$\begin{aligned} x &= \text{vec}\{x_1, \dots, x_N\}, & w &= \text{vec}\{w_1, \dots, w_N\} \\ v &= \text{vec}\{v_1, \dots, v_N\}, & Q &= \text{diag}\{Q_1, \dots, Q_N\} \\ R &= \text{diag}\{R_1, \dots, R_N\}, & H &= \text{diag}\{H_1, \dots, H_N\}, \end{aligned}$$

and

$$G = \begin{bmatrix} \mathbf{I} & 0 & & \\ -G_2 & \mathbf{I} & \ddots & \\ & \ddots & \ddots & 0 \\ & & -G_N & \mathbf{I} \end{bmatrix}$$

Then model (5.1) can be written in the form of (1.1)-(1.2), i.e.,

$$\begin{aligned}\mu &= Gx + w \\ z &= Hx + v,\end{aligned}\tag{5.2} \text{?fullStat?}$$

where  $x \in \mathbb{R}^{nN}$  is the entire state sequence of interest,  $w$  is corresponding process noise,  $z$  is the vector of all measurements,  $v$  is the measurement noise, and  $\mu$  is a vector of size  $nN$  with the first  $n$ -block equal to  $x_0$ , the initial state estimate, and the other blocks set to 0. This is precisely the problem (1.1)-(1.2) that began our study. The problem (1.3) becomes the classical Kalman smoothing problem with quadratic penalties. When the penalties arise from general PLQ densities, the general Kalman smoothing problem takes the form (4.3), studied in the previous section. The details are provided in the following remark.

**Remark 16** Suppose that the noises  $w$  and  $v$  in the model (5.2) are PLQ densities with means 0, variances  $Q$  and  $R$  (see Def. 12). Then, for suitable  $U_w, M_w, b_w, B_w$  and  $U_v, M_v, b_v, B_v$  and corresponding  $\rho_w$  and  $\rho_v$  we have

$$\begin{aligned}\mathbf{p}(w) &\propto \exp \left[ -\rho \left( U_w, M_w, b_w, B_w; Q^{-1/2} w \right) \right] \\ \mathbf{p}(v) &\propto \exp \left[ -\rho \left( U_v, M_v, b_v, B_v; R^{-1/2} v \right) \right]\end{aligned}\tag{5.3} \text{?kalmanDensities?}$$

while the MAP estimator of  $x$  in the model (5.2) is

$$\operatorname{argmin}_{x \in \mathbb{R}^{nN}} \left\{ \begin{aligned} &\rho \left[ U_w, M_w, b_w, B_w; Q^{-1/2} (Gx - \mu) \right] \\ &+ \rho \left[ U_v, M_v, b_v, B_v; R^{-1/2} (Hx - z) \right] \end{aligned} \right\}\tag{5.4} \text{?PLQsubproblem?}$$

If  $U_w$  and  $U_v$  are given as in (4.9), then the system (4.6) decomposes as

$$\begin{aligned}0 &= A_w^T u_w + s_w - a_w; & 0 &= A_v^T u_v + s_v - a_v \\ 0 &= s_w^T q_w; & 0 &= s_v^T q_v \\ 0 &= \tilde{b}_w + B_w Q^{-1/2} G d - M_w u_w - A_w q_w \\ 0 &= \tilde{b}_v - B_v R^{-1/2} H d - M_v u_v - A_v q_v \\ 0 &= G^T Q^{-1/2} B_w^T u_w - H^T R^{-1/2} B_v^T u_v \\ 0 &\leq s_w, s_v, q_w, q_v.\end{aligned}\tag{5.5} \text{?PLQFinalCondition?}$$

See the Appendix for details on deriving the KKT system. By further exploiting the decomposition shown in (5.1), we obtain the following theorem.

**Theorem 17 (PLQ Kalman smoother theorem)** Suppose that all  $w_k$  and  $v_k$  in the Kalman smoothing model (5.1) come from PLQ densities that satisfy

$$\operatorname{null}(M_k^w) \cap \operatorname{null}((A_k^w)^T) = \{0\}, \operatorname{null}(M_k^v) \cap \operatorname{null}((A_k^v)^T) = \{0\}, \forall k,\tag{5.6} \text{?NullPropertyKS?}$$

i.e. their corresponding penalties are finite-valued. Suppose further that the corresponding set  $\mathcal{F}_+$  from Theorem 14 is nonempty. Then (5.4) can be solved using an IP method, with computational complexity  $O[N(n^3 + m^3 + l)]$ , where  $l$  is the largest column dimension of the matrices  $\{A_k^v\}$  and  $\{A_k^w\}$ .

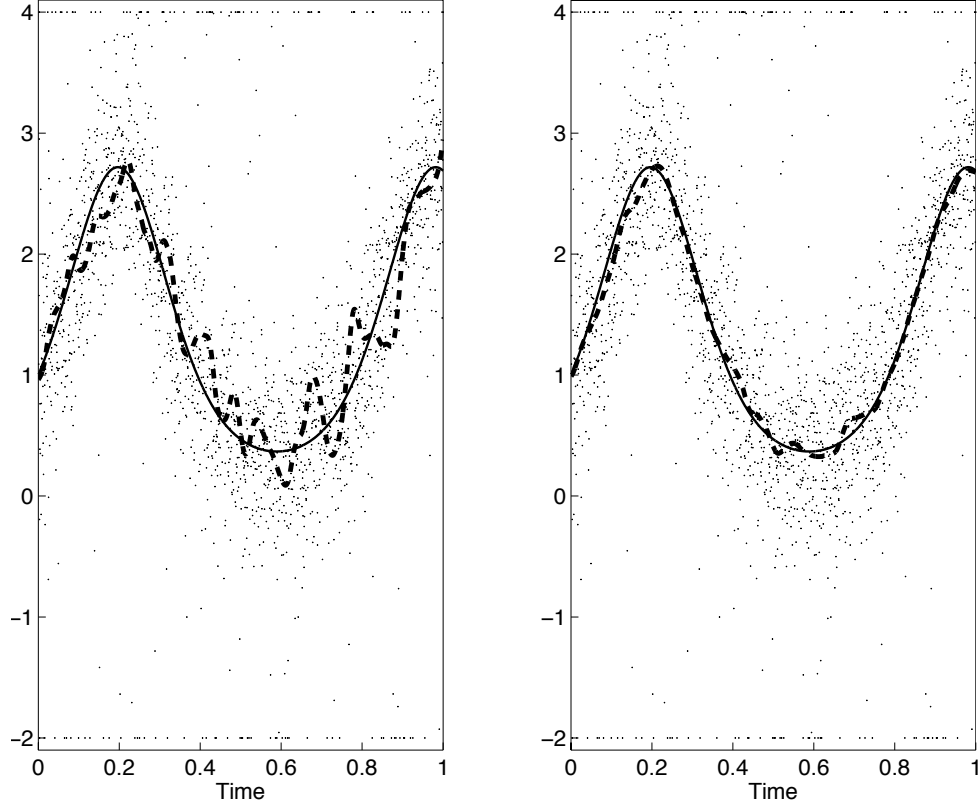


Figure 2: Simulation: measurements ( $\cdot$ ) with outliers plotted on axis limits (4 and  $-2$ ), true function (continuous line), smoothed estimate using either the quadratic loss (dashed line, left panel) or the Vapnik's  $\varepsilon$ -insensitive loss (dashed line, right panel)

Note that the first part of this theorem, the solvability of the problem using IP methods, already follows from Theorem 14. The main contribution of the result in the dynamical system context is the computational complexity. The proof is presented in the Appendix and shows that IP methods for solving (5.4) preserve the key block tridiagonal structure of the standard smoother. If the number of IP iterations is fixed ( $10 - 20$  are typically used in practice), general smoothing estimates can thus be computed in  $O[N(n^3 + m^3 + l)]$  time. Notice also that the number of required operations scales linearly with  $l$ , which represents the complexity of the PLQ density encoding.

## 6. Numerical example

### 6.1 Simulated data

In this section we use a simulated example to test the computational scheme described in the previous section. We consider the following function

$$f(t) = \exp[\sin(8t)]$$

taken from (Dinuzzo et al., 2007). Our aim is to reconstruct  $f$  starting from 2000 noisy samples collected uniformly over the unit interval. The measurement noise  $v_k$  was generated using a mixture of two Gaussian densities, with  $p = 0.1$  denoting the fraction from each Gaussian; i.e.,

$$v_k \sim (1 - p)\mathbf{N}(0, 0.25) + p\mathbf{N}(0, 25),$$

Data are displayed as dots in Fig. 2. Note that the purpose of the second component of the Gaussian mixture is to simulate outliers in the output data and that all the measurements exceeding vertical axis limits are plotted on upper and lower axis limits (4 and -2) to improve readability.

The initial condition  $f(0) = 1$  is assumed to be known, while the difference of the unknown function from the initial condition (i.e.  $f(\cdot) - 1$ ) is modeled as a Gaussian process given by an integrated Wiener process. This model captures the Bayesian interpretation of cubic smoothing splines (Wahba, 1990), and admits a two-dimensional state space representation where the first component of  $x(t)$ , which models  $f(\cdot) - 1$ , corresponds to the integral of the second state component, modelled as Brownian motion. To be more specific, letting  $\Delta t = 1/2000$ , the sampled version of the state space model (see (Jazwinski, 1970; Oksendal, 2005) for details) is defined by

$$\begin{aligned} G_k &= \begin{bmatrix} 1 & 0 \\ \Delta t & 1 \end{bmatrix}, & k = 2, 3, \dots, 2000 \\ H_k &= \begin{bmatrix} 0 & 1 \end{bmatrix}, & k = 1, 2, \dots, 2000 \end{aligned}$$

with the autocovariance of  $w_k$  given by

$$Q_k = \lambda^2 \begin{bmatrix} \Delta t & \frac{\Delta t^2}{2} \\ \frac{\Delta t^2}{2} & \frac{\Delta t^3}{3} \end{bmatrix}, \quad k = 1, 2, \dots, 2000,$$

where  $\lambda^2$  is an unknown scale factor to be estimated from the data.

We compare the performance of two Kalman smoothers. The first (classical) estimator uses a quadratic loss function to describe the negative log of the measurement noise density and contains only  $\lambda^2$  as unknown parameter. The second estimator is a Vapnik smoother relying on the  $\varepsilon$ -insensitive loss, and so depends on two unknown parameters:  $\lambda^2$  and  $\varepsilon$ . In both cases, the unknown parameters are estimated by means of a cross validation strategy where the 2000 measurements are randomly split into a training and a validation set of 1300 and 700 data points, respectively. The Vapnik smoother was implemented by exploiting the efficient computational strategy described in the previous section, see (Aravkin et al., 2011b) for specific implementation details. In this way, for each value of  $\lambda^2$  and  $\varepsilon$  contained in a  $10 \times 20$  grid on  $[0.01, 10000] \times [0, 1]$ , with  $\lambda^2$  logarithmically spaced, the function estimate was rapidly obtained by the new smoother applied to the training set. Then, the relative average prediction error on the validation set was computed, see Fig. 3.

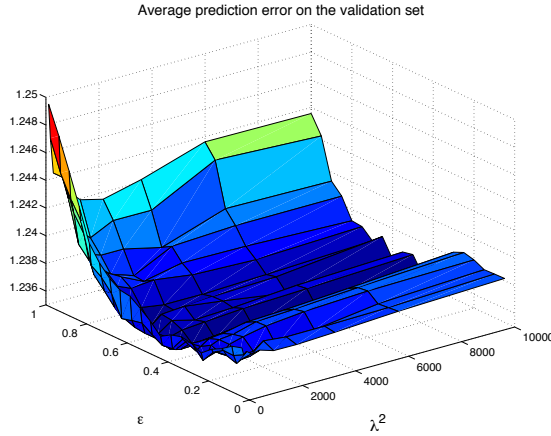


Figure 3: Estimation of the smoothing filter parameters using the Vapnik loss. Average prediction error on the validation data set as a function of the variance process  $\lambda^2$  and  $\varepsilon$ .

The parameters leading to the best prediction were  $\lambda^2 = 2.15 \times 10^3$  and  $\varepsilon = 0.45$ , which give a sparse solution defined by fewer than 400 support vectors. The value of  $\lambda^2$  for the classical Kalman smoother was then estimated following the same strategy described above. In contrast to the Vapnik penalty, the quadratic loss does not induce any sparsity, so that, in this case, the number of support vectors equals the size of the training set.

The left and right panels of Fig. 2 display the function estimate obtained using the quadratic and the Vapnik losses, respectively. It is clear that the estimate obtained using the quadratic penalty is heavily affected by the outliers. In contrast, as expected, the estimate coming from the Vapnik based smoother performs well over the entire time period, and is virtually unaffected by the presence of large outliers.

## 6.2 Real industrial data

Let us now consider real industrial data coming from Syncrude Canada Ltd, also analyzed in Liu et al. (2004). Oil production data is typically a multivariate time series capturing variables such as flow rate, pressure, particle velocity, and other observables. Because the data is proprietary, the exact nature of the variables is not known. The data from Liu et al. (2004) comprises two anonymized time series variables, called V14 and V36, that have been selected from the process data. Each time series consists of 936 measurements, collected at times  $[1, 2, \dots, 936]$  (see the top panels of Fig. 4). Due to the nature of production data, we hypothesize that the temporal profile of the variables is smooth and that the observations contain outliers, as suggested by the fact that some observations differ markedly from their neighbors, especially in the case of V14.

Our aim is to compare the prediction performance of two smoothers that rely on  $\ell_2$  and  $\ell_1$  measurement loss functions. For this purpose, we consider 100 Monte Carlo runs. During each run, data are randomly divided into three disjoint sets: training and a validation data sets, both of size 350, and a test set of size 236. We use the same state space model adopted in the previous subsection, with  $\Delta t = 1$ , and use a non-informative prior to model the initial condition of the system. The regulariza-

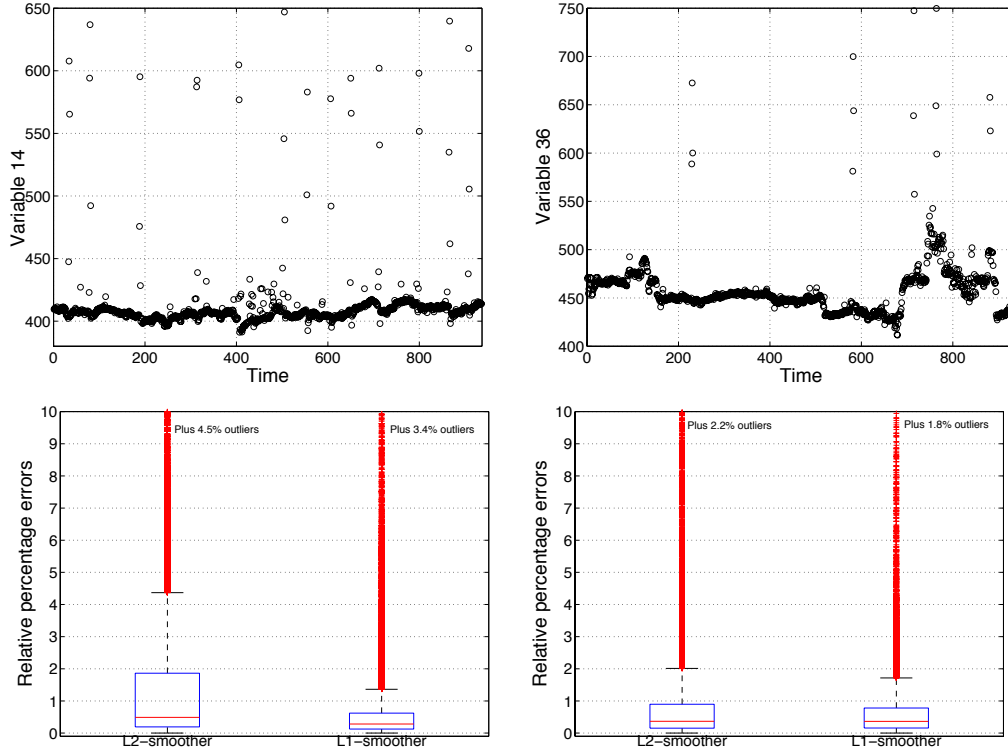


Figure 4: *Left panels*: data set for variable 14 (top) and relative percentage errors in the reconstruction of the test set obtained by Kalman smoothers based on the  $\ell_2$  and the  $\ell_1$  loss (bottom). *Right panels*: data set for variable 36 (top) and relative percentage errors in the reconstruction of the test set obtained by Kalman smoothers based on the  $\ell_2$  and the  $\ell_1$  loss (bottom).

tion parameter  $\gamma$  (equal to the inverse of  $\lambda^2$  assuming that the noise variance is 1) is chosen using standard cross validation techniques. For each value of  $\gamma$ , logarithmically spaced between 0.1 and 1000 (30 point grid), the smoothers are trained on the training set, and the  $\gamma$  chosen corresponds to the smoother that achieves the best prediction on the validation set. After estimating  $\gamma$ , the variable's profile is reconstructed for the entire time series (at all times  $[1, 2, \dots, 936]$ ), using the measurements contained in the union of the training and the validation data sets. Then, the prediction capability of the smoothers is evaluated by computing the 236 relative percentage errors (ratio of residual and observation times 100) in the reconstruction of the test set.

In Fig. 4 we display the boxplots of the overall 23600 relative errors stored after the 100 runs for V14 (bottom left panel) and V36 (bottom right panel). One can see that the  $\ell_1$ -Kalman smoother outperforms the classical one, especially in case of V14. This is not surprising, since in this case prediction is more difficult due to the larger numbers of outliers in the time series. In particular, for V14, the average percentage errors are 1.4% and 2.4% while, for V36, they are 1% and 1.2% using  $\ell_1$  and  $\ell_2$ , respectively.

## 7. Conclusions

We have presented a new theory for robust and sparse estimation using nonsmooth QS penalties. We give both primal and dual representations for these densities and show how to obtain closed form expressions using Euclidean projections. Using their dual representation, we first derived conditions allowing the interpretation of QS penalties as negative logs of true probability densities, thus establishing a statistical modeling framework. In this regard, the coercivity condition characterized in Th. 10 played a central role. This condition, necessary for the statistical interpretation, underscores the importance of an idea already useful in machine learning. Specifically, coercivity of the objective (1.4) is a fundamental prerequisite in sparse and robust estimation, as it precludes directions for which the sum of the loss and the regularizer are insensitive to large parameter changes. Thus, the condition for a QS penalty to be a negative log of a true density also ensures that the problem is well posed in the machine learning context, i.e. the learning machine has enough control over model complexity.

The QS class captures a variety of existing penalties used for both as misfit measures and as regularization functionals. We have also shown how to construct natural generalizations of these penalties within the QS class that are based on general norm and cone geometries. Moreover, we show how the structure of these functions can be understood through the use of Euclidean projections. Moreover, it is straightforward to use the presented results to design new formulations. Specifically, starting with the requisite *shape* of a new penalty, one can use results of Section 3 to obtain a standardized corresponding density, as well as the data structures  $U, M, B, b$  required to formulate and solve the optimization problem in Section 4. The statistical interpretation for these methods allows us to prescribe the mean and variance parameters of the corresponding model.

In the second part of the paper, we presented a broad computational approach to solving estimation problems (1.4) using interior point methods. In the process, we derived additional conditions that guarantee the successful implementation of IP methods to compute the estimator (1.4) when  $x$  and  $v$  come from PLQ densities (a broad subclass of QS penalties), and provided a theorem characterizing the convergence of IP methods for this class. The key condition required for the successful execution of IP iterations was a requirement on PLQ penalties to be finite valued, which implies non-degeneracy of the corresponding statistical distribution (the support cannot be contained in a lower-dimensional subspace). The statistical interpretation is thus strongly linked to the computational procedure.

We applied both the statistical framework and the computational approach to the broad class of state estimation problems in discrete-time dynamic systems, extending the classical formulations to allow dynamics and measurement noise to come from any PLQ densities. Moreover, we showed that the classical computational efficiency results can be preserved when the general IP approach is used in the state estimation context; specifically, PLQ Kalman smoothing can always be performed with a number of operations that is linear in the length of the time series, as in the quadratic case. The computational framework presented therefore allows the broad application of interior point methods to a wide class of smoothing problems of interest to practitioners. The powerful algorithmic scheme designed here, together with the breadth and significance of the new statistical framework presented, underscores the practical utility and flexibility of this approach. We believe that this perspective on modeling, robust/sparse estimation and Kalman smoothing will be useful in a number of applications in the years ahead.

In many contexts, it would be useful to estimate the parameters that define QS penalties; for exam-



ple the  $\kappa$  in the Huber penalty or the  $\varepsilon$  in the Vapnik penalty. In the numerical examples presented in this paper, we have relied on cross-validation to accomplish this task. An alternative method could be to compute the MAP points returned by our estimator for different filter parameters to gain information about the joint posterior of states and parameters. This strategy could help in designing a good proposal density for posterior simulation using e.g. particle smoothing filters (Ristic et al., 2004). We leave a detailed study of this approach to the QS modeling framework for future work.

## 8. Appendix

### 8.1 Proof of Theorem 3

Let  $\rho(y) = \rho(U, M, I, 0; y)$  so that  $\rho(U, M, B, b; y) = \rho(b + By)$ . Then  $\text{dom}(\rho(U, M, B, b; \cdot)) = B^{-1}(\text{dom}(\rho) - b)$ , hence the theorem follows if it can be shown that  $\text{bar}(U) + \text{Ran}(M) \subset \text{dom}(\rho) \subset [U^\infty \cap \text{null}(M)]^\circ$  with equality when  $\text{bar}(U) + \text{Ran}(M)$  is closed. Observe that if there exists  $w \in U^\infty \cap \text{null}(M)$  such that  $\langle y, w \rangle > 0$ , then trivially  $\rho(y) = +\infty$  so  $y \notin \text{dom}(\rho)$ . Consequently,  $\text{dom}(\rho) \subset [U^\infty \cap \text{null}(M)]^\circ$ . Next let  $y \in \text{bar}(U) + \text{Ran}(M)$ , then there is a  $v \in \text{bar}(U)$  and  $w$  such that  $y = v + Mw$ . Hence

$$\begin{aligned} \sup_{u \in U} [\langle u, y \rangle - \tfrac{1}{2} \langle u, Mu \rangle] &= \sup_{u \in U} [\langle u, v + Mw \rangle - \tfrac{1}{2} \langle u, Mu \rangle] \\ &= \sup_{u \in U} [\langle u, v \rangle + \tfrac{1}{2} w^T M w - \tfrac{1}{2} (w - u)^T M (w - u)] \\ &\leq \delta^*(v | U) + \tfrac{1}{2} w^T M w < \infty. \end{aligned}$$

Hence  $\text{bar}(U) + \text{Ran}(M) \subset \text{dom}(\rho)$ .

If the set  $\text{bar}(U) + \text{Ran}(M)$  is closed, then so is the set  $\text{bar}(U)$ . Therefore, by (Rockafellar, 1970, Corollary 14.2.1),  $(U^\infty)^\circ = \text{bar}(U)$ , and, by (Rockafellar, 1970, Corollary 16.4.2),  $[U^\infty \cap \text{null}(M)]^\circ = \text{bar}(U) + \text{Ran}(M)$ , which proves the result.

The polyhedral case  $\text{bar}(U)$  is a polyhedral convex set, and the sum of such sets is also a polyhedral convex set (Rockafellar, 1970, Corollary 19.3.2).

### 8.2 Proof of Theorem 7

To see the first equation in (2.4) write  $\rho(y) = \sup_u [\langle y, u \rangle - (\tfrac{1}{2} \|L^T u\|_2^2 + \delta(u | U))]$ , and then apply the calculus of convex conjugate functions (Rockafellar, 1970, Section 16) to find that

$$(\tfrac{1}{2} \|L^T \cdot\|_2^2 + \delta(\cdot | U))^*(y) = \inf_{s \in \mathbb{R}^k} [\tfrac{1}{2} \|s\|_2^2 + \delta^*(y - Ls | U)].$$

The second equivalence in (2.4) follows from (Rockafellar, 1970, Theorem 14.5).

For the remainder, we assume that  $M$  is positive definite. In this case it is easily shown that  $(MU)^\circ = M^{-1}U^\circ$ . Hence, by (Rockafellar, 1970, Theorem 14.5),  $\gamma(\cdot | MU) = \delta^*(\cdot | M^{-1}U^\circ)$ . We use these facts freely throughout the proof.

The formula (2.5) follows by observing that

$$\tfrac{1}{2} \|s\|_2^2 + \delta^*(y - Ls | U) = \tfrac{1}{2} \|L^{-T} s\|_M^2 + \delta^*(M^{-1}y - L^{-T} s | MU)$$

and then making the substitution  $v = L^{-T} s$ . To see (2.6), note that the optimality conditions for (2.5) are  $Ms \in \partial \delta^*(M^{-1}y - s | MU)$ , or equivalently,  $M^{-1}y - s \in N(Ms | MU)$ , i.e.  $s \in U$  and

$$\langle M^{-1}y - s, u - s \rangle_M = \langle M^{-1}y - s, M(u - s) \rangle \leq 0 \quad \forall u \in U,$$

which, by (2.3), tells us that  $s = P_M(M^{-1}y|U)$ . Plugging this into (2.5) gives (2.6).

Using the substitution  $v = Ls$ , the argument showing (2.7) and (2.8) differs only slightly from that for (2.5) and (2.5) and so is omitted.

The formula (2.9) follows by completing the square in the  $M$ -norm in the definition (2.1):

$$\begin{aligned}\langle y, u \rangle - \frac{1}{2} \langle u, Mu \rangle &= \langle M^{-1}y, u \rangle_M - \frac{1}{2} \langle u, u \rangle_M \\ &= \frac{1}{2} y^T M^{-1}y - \frac{1}{2} [\langle M^{-1}y, M^{-1}y \rangle_M - 2 \langle M^{-1}y, u \rangle_M + \langle u, u \rangle_M] \\ &= \frac{1}{2} y^T M^{-1}y - \frac{1}{2} \|M^{-1}y - u\|_M^2.\end{aligned}$$

The result as well as (2.10) now follow from Theorem 6. Both (2.11) and (2.12) follow similarly by completing the square in the  $M^{-1}$ -norm.

### 8.3 Proof of Theorem 9

First we will show that if  $\rho$  is convex coercive, then for any  $\bar{x} \in \operatorname{argmin} f \neq \emptyset$ , there exist constants  $R$  and  $K > 0$  such that

$$\rho(x) \geq \rho(\bar{x}) + K\|x - \bar{x}\| \quad \forall x \notin R\mathbb{B}. \quad (8.1) \text{ ?boundRho?}$$

Without loss of generality, we can assume that  $0 = \rho(0) = \inf \rho$ . Otherwise, replace  $\rho(x)$  by  $\hat{\rho}(x) = \rho(x + \bar{x}) - \rho(\bar{x})$ , where  $\bar{x}$  is any global minimizer of  $\rho$ .

Let  $\alpha > 0$ . Since  $\rho$  is coercive, there exists  $R$  such that  $\operatorname{lev}_\rho(\alpha) \subset R\mathbb{B}$ . We will show that  $\frac{\alpha}{R}\|x\| \leq \rho(x)$  for all  $x \notin R\mathbb{B}$ .

Indeed, for all  $x \neq 0$ , we have  $\rho(\frac{R}{\|x\|}x) \geq \alpha$ . Therefore, if  $x \notin R\mathbb{B}$ , then  $0 < \frac{R}{\|x\|} < 1$ , and we have

$$\frac{\alpha}{R}\|x\| \leq \frac{\|x\|}{R} \rho\left(\frac{R}{\|x\|}x\right) \leq \frac{\|x\|}{R} \frac{R}{\|x\|} \rho(x) = \rho(x).$$

Then by (8.1),

$$\begin{aligned}\int \exp(-\rho(x)) dx &= \int_{\bar{x}+R\mathbb{B}} \exp(-\rho(x)) dx + \int_{\|x-\bar{x}\|>R} \exp(-\rho(x)) dx \\ &\leq C_1 + C_2 \int_{\|x-\bar{x}\|>R} \exp(-K\|x-\bar{x}\|) dx < \infty.\end{aligned}$$

### 8.4 Proof of Theorem 10

First observe that  $B^{-1}[\operatorname{cone}(U)]^\circ = [B^T \operatorname{cone}(U)]^\circ$  by (Rockafellar, 1970, Corollary 16.3.2).

Suppose that  $\hat{y} \in B^{-1}[\operatorname{cone}(U)]^\circ$ , and  $\hat{y} \neq 0$ . Then  $B\hat{y} \in \operatorname{cone}(U)$ , and  $B\hat{y} \neq 0$  since  $B$  is injective, and we have

$$\begin{aligned}\rho(t\hat{y}) &= \sup_{u \in U} \langle b + tB\hat{y}, u \rangle - \frac{1}{2} u^T M u \\ &= \sup_{u \in U} \langle b, u \rangle - \frac{1}{2} u^T M u + t \langle B\hat{y}, u \rangle \\ &\leq \sup_{u \in U} \langle b, u \rangle - \frac{1}{2} u^T M u \\ &\leq \rho(U, M, 0, I; b),\end{aligned}$$

so  $\rho(t\hat{y})$  stays bounded even as  $t \rightarrow \infty$ , and so  $\rho$  cannot be coercive.

Conversely, suppose that  $\rho$  is not coercive. Then we can find a sequence  $\{y_k\}$  with  $\|y_k\| > k$  and a constant  $P$  so that  $\rho(y_k) \leq P$  for all  $k > 0$ . Without loss of generality, we may assume that  $\frac{y_k}{\|y_k\|} \rightarrow \bar{y}$ .

Then by definition of  $\rho$ , we have for all  $u \in U$

$$\begin{aligned} \langle b + By_k, u \rangle - \frac{1}{2} u^T M u &\leq P \\ \langle b + By_k, u \rangle &\leq P + \frac{1}{2} u^T M u \\ \left\langle \frac{b + By_k}{\|y_k\|}, u \right\rangle &\leq \frac{P}{\|y_k\|} + \frac{1}{2\|y_k\|} u^T M u \end{aligned}$$

Note that  $\bar{y} \neq 0$ , so  $B\bar{y} \neq 0$ . When we take the limit as  $k \rightarrow \infty$ , we get  $\langle B\bar{y}, u \rangle \leq 0$ . From this inequality we see that  $B\bar{y} \in [\text{cone}(U)]^\circ$ , and so  $\bar{y} \in B^{-1}[\text{cone}(U)]^\circ$ .

## 8.5 Proof of Theorem 14

**Proof** (i) Using standard elementary row operations, reduce the matrix

$$F_\gamma^{(1)} := \begin{bmatrix} I & 0 & A^T & 0 \\ D(q) & D(s) & 0 & 0 \\ 0 & -A & -M & B \\ 0 & 0 & B^T & 0 \end{bmatrix} \quad (8.2) \text{?rKKTder?}$$

to

$$\begin{bmatrix} I & 0 & A^T & 0 \\ 0 & D(s) & -D(q)A^T & 0 \\ 0 & 0 & -T & B \\ 0 & 0 & B^T & 0 \end{bmatrix},$$

where  $T = M + AD(q)D(s)^{-1}A^T$ . The matrix  $T$  is invertible since  $\text{null}(M) \cap \text{null}(C^T) = \{0\}$ . Hence, we can further reduce this matrix to the block upper triangular form

$$\begin{bmatrix} I & 0 & A^T & 0 \\ 0 & D(s) & -D(q)C^T & 0 \\ 0 & 0 & -T & B \\ 0 & 0 & 0 & -B^T T^{-1} B \end{bmatrix}.$$

Since  $B$  is injective, the matrix  $B^T T^{-1} B$  is also invertible. Hence this final block upper triangular is invertible proving Part (i).

(ii) Let  $(s, q) \in \widehat{\mathcal{F}}_+$  and choose  $(u_i, y_i)$  so that  $(s, q, u_i, y_i) \in \mathcal{F}_+$  for  $i = 1, 2$ . Set  $u := u_1 - u_2$  and  $y := y_1 - y_2$ . Then, by definition,

$$0 = A^T u, \quad 0 = By - Mu, \quad \text{and} \quad 0 = B^T u. \quad (8.3) \text{?null space contr}$$

Multiplying the second of these equations on the left by  $u$  and utilizing the third as well as the positive semi-definiteness of  $M$ , we find that  $Mu = 0$ . Hence,  $u \in \text{null}(M) \cap \text{null}(A^T) = \{0\}$ , and so  $By = 0$ . But then  $y = 0$  as  $B$  is injective.

(iii) Let  $(\hat{s}, \hat{q}, \hat{u}, \hat{y}) \in \mathcal{F}_+$  and  $(s, q, u, y) \in \mathcal{F}_+(\tau)$ . Then, by (4.6),

$$\begin{aligned} (s - \hat{s})^T (q - \hat{q}) &= [(a - A^T u) - (a - A^T \hat{u})]^T (q - \hat{q}) \\ &= (\hat{u} - u)^T (Aq - A\hat{q}) \\ &= (\hat{u} - u)^T [(b + By - Mu) - (b + B\hat{y} - M\hat{u})] \\ &= (\hat{u} - u)^T M(\hat{u} - u) \\ &\geq 0. \end{aligned}$$

Hence,

$$\tau + \hat{s}^T \hat{q} \geq s^T y + \hat{s}^T \hat{q} \geq s^T \hat{y} + y^T \hat{s} \geq \xi \| (s, q) \|_1,$$

where  $\xi = \min \{ \hat{s}_i, \hat{q}_i \mid i = 1, \dots, \ell \} > 0$ . Therefore, the set

$$\widehat{\mathcal{F}}_+(\tau) = \{ (s, q) \mid (s, q, u, y) \in \mathcal{F}_+(\tau) \}$$

is bounded. Now suppose the set  $\mathcal{F}_+(\tau)$  is not bounded. Then there exists a sequence  $\{ (s_v, q_v, u_v, y_v) \} \subset \mathcal{F}_+(\tau)$  such that  $\| (s_v, q_v, u_v, y_v) \| \uparrow +\infty$ . Since  $\widehat{\mathcal{F}}_+(\tau)$  is bounded, we can assume that  $\| (u_v, y_v) \| \uparrow +\infty$  while  $\| (s_v, q_v) \|$  remains bounded. With no loss in generality, we may assume that there exists  $(u, y) \neq (0, 0)$  such that  $(u_v, y_v) / \| (u_v, y_v) \| \rightarrow (u, y)$ . By dividing (4.6) by  $\| (u_v, y_v) \|$  and taking the limit, we find that (8.3) holds. But then, as in (8.3),  $(u, y) = (0, 0)$ . This contradiction yields the result.

(iv) We first show existence. This follows from a standard continuation argument. Let  $(\hat{s}, \hat{q}, \hat{u}, \hat{y}) \in \mathcal{F}_+$  and  $v \in \mathbb{R}_{++}^\ell$ . Define

$$F(s, q, u, y, t) = \begin{bmatrix} s + A^T u - a \\ D(q)D(s)\mathbf{1} - [(1-t)\hat{v} + tv] \\ By - Mu - Aq \\ B^T u + b \end{bmatrix}, \quad (8.4) \text{homotopy } F?$$

where  $\hat{g} := (\hat{s}_1 \hat{y}_1, \dots, \hat{s}_\ell \hat{y}_\ell)^T$ . Note that

$$F(\hat{s}, \hat{q}, \hat{u}, \hat{y}, 0) = 0 \text{ and, by Part (i), } \nabla_{(s, q, u, y)} F(\hat{s}, \hat{q}, \hat{u}, \hat{y}, 0)^{-1} \text{ exists.}$$

The Implicit Function Theorem implies that there is a  $\tilde{t} > 0$  and a differentiable mapping  $t \mapsto (s(t), q(t), u(t), y(t))$  on  $[0, \tilde{t})$  such that

$$F[s(t), q(t), u(t), y(t), t] = 0 \text{ on } [0, \tilde{t}).$$

Let  $\bar{t} > 0$  be the largest such  $\tilde{t}$  on  $[0, 1]$ . Since

$$\{ [s(t), q(t), u(t), y(t)] \mid t \in [0, \bar{t}) \} \subset \mathcal{F}_+(\bar{\tau}),$$

where  $\bar{\tau} = \max \{ \mathbf{1}^T \hat{g}, \mathbf{1}^T \bar{g} \}$ , Part (iii) implies that there is a sequence  $t_i \rightarrow \bar{t}$  and a point  $(\bar{s}, \bar{q}, \bar{u}, \bar{y})$  such that  $[s(t_i), q(t_i), u(t_i), y(t_i)] \rightarrow (\bar{s}, \bar{q}, \bar{u}, \bar{y})$ . By continuity  $F(\bar{s}, \bar{q}, \bar{u}, \bar{y}, \bar{t}) = 0$ . If  $\bar{t} = 1$ , we are done; otherwise, apply the Implicit Function Theorem again at  $(\bar{s}, \bar{q}, \bar{u}, \bar{y}, \bar{t})$  to obtain a contradiction to the maximality of  $\bar{t}$ .

We now show uniqueness. By Part (ii), we need only establish the uniqueness of  $(s, q)$ . Let  $(s^v, q^v) \in \widehat{\mathcal{F}}_+$  be such that  $g = (s_{j(1)} q_{j(1)}, s_{j(2)} q_{j(2)}, \dots, s_{j(\ell)} q_{j(\ell)})^T$ , where  $s_{j(i)}$  denotes the  $i$ th element of  $s_j$ , and  $j = 1, 2$ . As in Part (iii), we have  $(s_1 - s_2)^T (q_1 - q_2) = (u_1 - u_2)^T M (u_1 - u_2) \geq 0$ , and, for each  $i = 1, \dots, \ell$ ,  $s_{1(i)} q_{1(i)} = s_{2(i)} q_{2(i)} = g_i > 0$ . If  $(s_1, q_1) \neq (s_2, q_2)$ , then, for some  $i \in \{1, \dots, \ell\}$ ,  $(s_{1(i)} - s_{2(i)})(q_{1(i)} - q_{2(i)}) \geq 0$  and either  $s_{1(i)} \neq s_{2(i)}$  or  $q_{1(i)} \neq q_{2(i)}$ . If  $s_{1(i)} > s_{2(i)}$ , then  $q_{1(i)} \geq q_{2(i)} > 0$  so that  $g_i = s_{1(i)} q_{1(i)} > s_{2(i)} q_{2(i)} = g_i$ , a contradiction. So with out loss in generality (by exchanging  $(s_1, q_1)$  with  $(s_2, q_2)$  if necessary), we must have  $q_{1(i)} > q_{2(i)}$ . But then  $s_{1(i)} \geq s_{2(i)} > 0$ , so that again  $g_i = s_{1(i)} q_{1(i)} > s_{2(i)} q_{2(i)} = g_i$ , and again a contradiction. Therefore,  $(s, q)$  is unique.

(v) Apply Part (iv) to get a point on the central path and then use the continuation argument to trace out the central path. The differentiability follows from the implicit function theorem.

(vi) Part (iii) allows us to apply a standard compactness argument to get the existence of cluster points and the continuity of  $F_\gamma(s, q, u, y)$  in all of its arguments including  $\gamma$  implies that all of these cluster points solve (4.6).  $\blacksquare$

## 8.6 Details for Remark 16

The Lagrangian for (5.4) for feasible  $(x, u_w, u_v)$  is

$$L(x, u_w, u_v) = \left\langle \begin{bmatrix} \tilde{b}_w \\ \tilde{b}_v \end{bmatrix}, \begin{bmatrix} u_w \\ u_v \end{bmatrix} \right\rangle - \frac{1}{2} \begin{bmatrix} u_w \\ u_v \end{bmatrix}^T \begin{bmatrix} M_w & 0 \\ 0 & M_v \end{bmatrix} \begin{bmatrix} u_w \\ u_v \end{bmatrix} - \left\langle \begin{bmatrix} u_w \\ u_v \end{bmatrix}, \begin{bmatrix} -B_w Q^{-1/2} G \\ B_v R^{-1/2} H \end{bmatrix} x \right\rangle \quad (8.5) \text{?PLQLagrangian?}$$

where  $\tilde{b}_w = b_w - B_w Q^{-1/2} \tilde{x}_0$  and  $\tilde{b}_v = b_v - B_v R^{-1/2} \tilde{z}$ . The associated optimality conditions for feasible  $(x, u_w, u_v)$  are given by

$$\begin{aligned} G^T Q^{-1/2} B_w^T \tilde{u}_w - H^T R^{-1/2} B_v^T \tilde{u}_v &= 0 \\ \tilde{b}_w - M_w \tilde{u}_w + B_w Q^{-1/2} G \tilde{x} &\in N_{U_w}(\tilde{u}_w) \\ \tilde{b}_v - M_v \tilde{u}_v - B_v R^{-1/2} H \tilde{x} &\in N_{U_v}(\tilde{u}_v), \end{aligned} \quad (8.6) \text{?PLQOptimalityCon}$$

where  $N_C(r)$  denotes the normal cone to the set  $C$  at the point  $r$  (see (Rockafellar, 1970) for details).

Since  $U_w$  and  $U_v$  are polyhedral, we can derive explicit representations of the normal cones  $N_{U_w}(\tilde{u}_w)$  and  $N_{U_v}(\tilde{u}_v)$ . For a polyhedral set  $U \subset \mathbb{R}^m$  and any point  $\bar{u} \in U$ , the normal cone  $N_U(\bar{u})$  is polyhedral. Indeed, relative to any representation

$$U = \{u \mid A^T u \leq a\}$$

and the active index set  $I(\bar{u}) := \{i \mid \langle A_i, \bar{u} \rangle = a_i\}$ , where  $A_i$  denotes the  $i$ th column of  $A$ , we have

$$N_U(\bar{u}) = \left\{ q_1 A_1 + \cdots + q_m A_m \mid \begin{array}{l} q_i \geq 0 \text{ for } i \in I(\bar{u}) \\ q_i = 0 \text{ for } i \notin I(\bar{u}) \end{array} \right\}. \quad (8.7) \text{?NormalRep?}$$

Using (8.7), Then we may rewrite the optimality conditions (8.6) more explicitly as

$$\begin{aligned} G^T Q^{-1/2} B_w^T \tilde{u}_w - H^T R^{-1/2} B_v^T \tilde{u}_v &= 0 \\ \tilde{b}_w - M_w \tilde{u}_w + B_w Q^{-1/2} G \tilde{d} &= A_w q_w \\ \tilde{b}_v - M_v \tilde{u}_v - B_v R^{-1/2} H \tilde{d} &= A_v q_v \\ \{q_v \geq 0 \mid q_{v(i)} &= 0 \text{ for } i \notin I(\tilde{u}_v)\} \\ \{q_w \geq 0 \mid q_{w(i)} &= 0 \text{ for } i \notin I(\tilde{u}_w)\} \end{aligned} \quad (8.8) \text{?PLQExpandedCondi}$$

where  $q_{v(i)}$  and  $q_{w(i)}$  denote the  $i$ th elements of  $q_v$  and  $q_w$ . Define slack variables  $s_w \geq 0$  and  $s_v \geq 0$  as follows:

$$\begin{aligned} s_w &= a_w - A_w^T \tilde{u}_w \\ s_v &= a_v - A_v^T \tilde{u}_v. \end{aligned} \quad (8.9) \text{?slack?}$$

Note that we know the entries of  $q_{w(i)}$  and  $q_{v(i)}$  are zero if and only if the corresponding slack variables  $s_{v(i)}$  and  $s_{w(i)}$  are nonzero, respectively. Then we have  $q_w^T s_w = q_v^T s_v = 0$ . These equations are known as the complementarity conditions. Together, all of these equations give system (5.5).

## 8.7 Proof of Theorem 17

IP methods apply a damped Newton iteration to find the solution of the relaxed KKT system  $F_\gamma = 0$ , where

$$F_\gamma \begin{pmatrix} s_w \\ s_v \\ q_w \\ q_v \\ u_w \\ u_v \\ x \end{pmatrix} = \begin{bmatrix} A_w^T u_w + s_w - a_w \\ A_v^T u_v + s_v - a_v \\ D(q_w)D(s_w)\mathbf{1} - \gamma\mathbf{1} \\ D(q_v)D(s_v)\mathbf{1} - \gamma\mathbf{1} \\ \tilde{b}_w + B_w Q^{-1/2} G d - M_w u_w - A_w q_w \\ \tilde{b}_v - B_v R^{-1/2} H d - M_v u_v - A_v q_v \\ G^T Q^{-T/2} B_w^T u_w - H^T R^{-T/2} B_v^T u_v \end{bmatrix}.$$

This entails solving the system

$$F_\gamma^{(1)} \begin{pmatrix} s_w \\ s_v \\ q_w \\ q_v \\ u_w \\ u_v \\ x \end{pmatrix} = -F_\gamma \begin{pmatrix} s_w \\ s_v \\ q_w \\ q_v \\ u_w \\ u_v \\ x \end{pmatrix}, \quad (8.10) \text{?NewtonSystem?}$$

where the derivative matrix  $F_\gamma^{(1)}$  is given by

$$\begin{bmatrix} I & 0 & 0 & 0 & (A_w)^T & 0 & 0 \\ 0 & I & 0 & 0 & 0 & (A_v)^T & 0 \\ D(q_w) & 0 & D(s_w) & 0 & 0 & 0 & 0 \\ 0 & D(q_v) & 0 & D(s_v) & 0 & 0 & 0 \\ 0 & 0 & -A_w & 0 & -M_w & 0 & B_w Q^{-1/2} G \\ 0 & 0 & 0 & -A_v & 0 & -M_v & -B_v R^{-1/2} H \\ 0 & 0 & 0 & 0 & G^T Q^{-T/2} B_w^T & -H^T R^{-T/2} B_v^T & 0 \end{bmatrix} \quad (8.11) \text{?Fprime?}$$

We now show the row operations necessary to reduce the matrix  $F_\gamma^{(1)}$  in (8.11) to upper block triangular form. After each operation, we show only the row that was modified.

$$\begin{aligned} \text{row}_3 &\leftarrow \text{row}_3 - D(q_w) \text{row}_1 \\ [0 \quad 0 \quad D(s_w) \quad 0 \quad -D(q_w)A_w^T \quad 0 \quad 0] \\ \text{row}_4 &\leftarrow \text{row}_4 - D(q_v) \text{row}_2 \\ [0 \quad 0 \quad 0 \quad D(s_v) \quad 0 \quad -D(q_v)A_v^T \quad 0] \\ \text{row}_5 &\leftarrow \text{row}_5 + A_w D(s_w)^{-1} \text{row}_3 \\ [0 \quad 0 \quad 0 \quad 0 \quad -T_w \quad 0 \quad B_w Q^{-1/2} G] \\ \text{row}_6 &\leftarrow \text{row}_6 + A_v D(s_v)^{-1} \text{row}_4 \\ [0 \quad 0 \quad 0 \quad 0 \quad 0 \quad -T_v \quad -B_v R^{-1/2} H] \end{aligned}$$

In the above expressions,

$$\begin{aligned} T_w &:= M_w + A_w D(s_w)^{-1} D(q_w) A_w^T \\ T_v &:= M_v + A_v D(s_v)^{-1} D(q_v) A_v^T, \end{aligned} \quad (8.12) \text{?KalmanT?}$$

where  $D(s_w)^{-1}D(q_w)$  and  $D(s_v)^{-1}D(q_v)$  are always full-rank diagonal matrices, since the vectors  $s_w, q_w, s_v, q_v$ . Matrices  $T_w$  and  $T_v$  are invertible as long as the PLQ densities for  $w$  and  $v$  satisfy (4.10).

**Remark 18 (block diagonal structure of  $T$  in i.d. case)** Suppose that  $y$  is a random vector,  $y = \text{vec}(\{y_k\})$ , where each  $y_i$  is itself a random vector in  $\mathbb{R}^{m(i)}$ , from some PLQ density  $\mathbf{p}(y_i) \propto \exp[-c_2 \rho(U_i, M_i, 0, I; \cdot)]$ , and all  $y_i$  are independent. Let  $U_i = \{u : A_i^T u \leq a_i\}$ . Then the matrix  $T_\rho$  is given by  $T_\rho = M + ADA^T$  where  $M = \text{diag}[M_1, \dots, M_N]$ ,  $A = \text{diag}[A_1, \dots, A_N]$ ,  $D = \text{diag}[D_1, \dots, D_N]$ , and  $\{D_i\}$  are diagonal with positive entries. Moreover,  $T_\rho$  is block diagonal, with  $i$ th diagonal block given by  $M_i + A_i D_i A_i^T$ .

From Remark 18, the matrices  $T_w$  and  $T_v$  in (8.12) are block diagonal provided that  $\{w_k\}$  and  $\{v_k\}$  are independent vectors from any PLQ densities.

We now finish the reduction of  $F_\gamma^{(1)}$  to upper block triangular form:

$$\text{row}_7 \leftarrow \text{row}_7 + \left(G^T Q^{-T/2} B_w^T T_w^{-1}\right) \text{row}_5 - \left(H^T R^{-T/2} B_v^T T_v^{-1}\right) \text{row}_6$$

$$\begin{bmatrix} I & 0 & 0 & 0 & (A_w)^T & 0 & 0 \\ 0 & I & 0 & 0 & 0 & (A_v)^T & 0 \\ 0 & 0 & S_w & 0 & -Q_w(A_w)^T & 0 & 0 \\ 0 & 0 & 0 & S_v & 0 & -Q_v(A_v)^T & 0 \\ 0 & 0 & 0 & 0 & -T_w & 0 & B_w Q^{-1/2} G \\ 0 & 0 & 0 & 0 & 0 & -T_v & -B_v R^{-1/2} H \\ 0 & 0 & 0 & 0 & 0 & 0 & \Omega \end{bmatrix}$$

where

$$\Omega = \Omega_G + \Omega_H = G^T Q^{-T/2} B_w^T T_w^{-1} B_w Q^{-1/2} G + H^T R^{-T/2} B_v^T T_v^{-1} B_v R^{-1/2} H. \quad (8.13) \text{?}\Omega_{\text{Matrix?}}$$

Note that  $\Omega$  is symmetric positive definite. Note also that  $\Omega$  is block tridiagonal, since

1.  $\Omega_H$  is block diagonal.
2.  $Q^{-T/2} B_w^T T_w^{-1} B_w Q^{-1/2}$  is block diagonal, and  $G$  is block bidiagonal, hence  $\Omega_G$  is block tridiagonal.

Solving system (8.10) requires inverting the block diagonal matrices  $T_v$  and  $T_w$  at each iteration of the damped Newton's method, as well as solving an equation of the form  $\Omega \Delta x = \rho$ . The matrices  $T_v$  and  $T_w$  are block diagonal, with sizes  $Nn$  and  $Nm$ , assuming  $m$  measurements at each time point. Given that they are invertible (see (4.10)), these inversions take  $O(Nn^3)$  and  $O(Nm^3)$  time. Since  $\Omega$  is block tridiagonal, symmetric, and positive definite,  $\Omega \Delta x = \rho$  can be solved in  $O(Nn^3)$  time using the block tridiagonal algorithm in (Bell, 2000). The remaining four back solves required to solve (8.10) can each be done in  $O(Nl)$  time, where we assume that  $A_{v(k)} \in \mathbb{R}^{n \times l}$  and  $A_{w(k)} \in \mathbb{R}^{m \times l}$  at each time point  $k$ .

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